

Tools for special functions and special numbers

Graduate Student Colloquium
Tulane University, New Orleans

Armin Straub

October 15, 2013

University of Illinois
at Urbana–Champaign

&

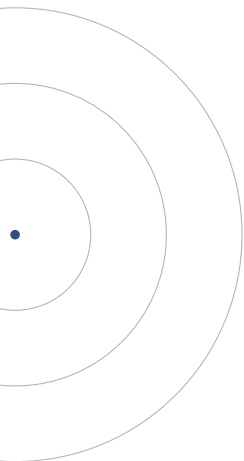
Max-Planck-Institut
für Mathematik, Bonn

ISC — PSLQ — OEIS — CAD — WZ

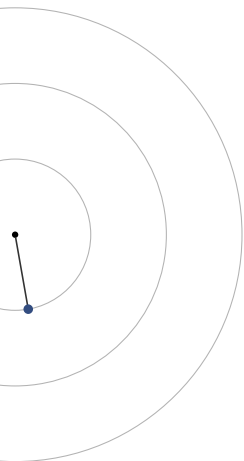
THE TOOLS TODAY

- ISC** Inverse Symbolic Calculator
- PSLQ** Lattice Reduction Algorithm
- OEIS** On-Line Encyclopedia of Integer Sequences
- CAD** Cylindrical Algebraic Decomposition
- WZ** Wilf–Zeilberger Theory

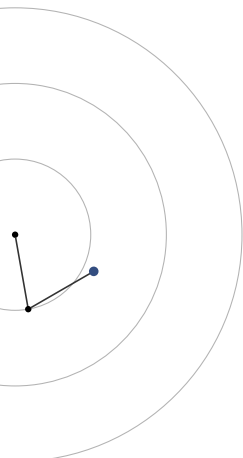
- We study random walks in the plane consisting of n steps. Each step is of length 1 and is taken in a randomly chosen direction.



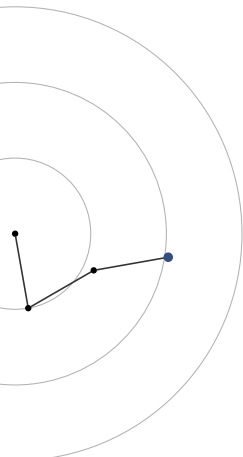
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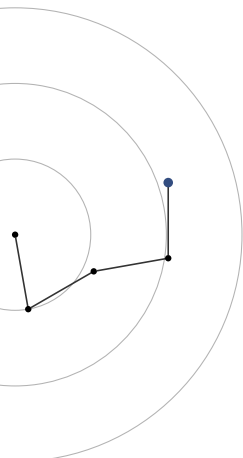
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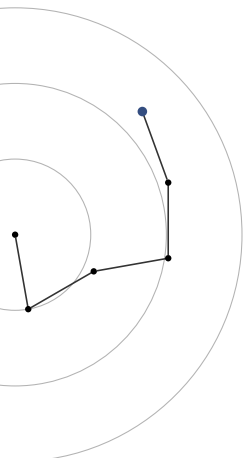
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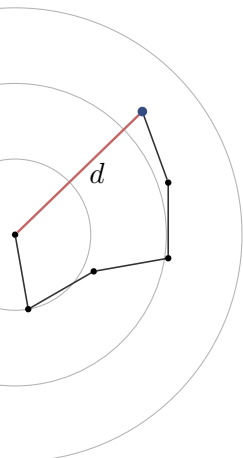
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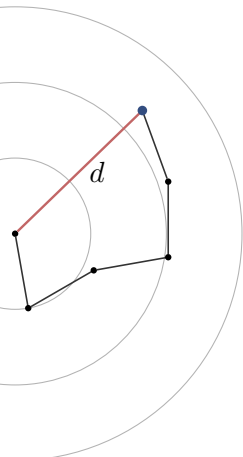


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- We study random walks in the plane consisting of n steps. Each step is of length 1 and is taken in a randomly chosen direction.
- We are interested in the distance traveled in n steps.

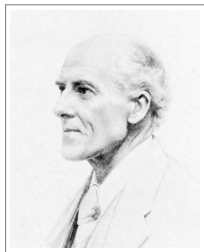
Q For instance, how large is this distance on average?

- Probability density: $p_n(x)$

Random walks are only about 100 years old

- Karl Pearson asked for $p_n(x)$ in Nature in 1905.

This famous question coined the term **random walk**.



The Problem of the Random Walk.

CAN any of your readers refer me to a work wherein I should find a solution of the following problem, or failing the knowledge of any existing solution provide me with an original one? I should be extremely grateful for aid in the matter.

A man starts from a point O and walks l yards in a straight line; he then turns through any angle whatever and walks another l yards in a second straight line. He repeats this process n times. I require the probability that after these n stretches he is at a distance between r and $r + \delta r$ from his starting point, O.

The problem is one of considerable interest, but I have only succeeded in obtaining an integrated solution for *two* stretches. I think, however, that a solution ought to be found, if only in the form of a series in powers of $1/n$, when n is large.

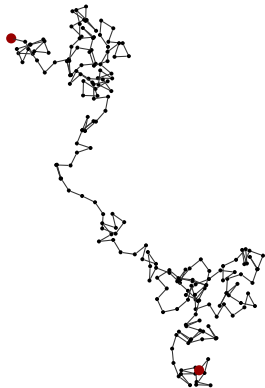
KARL PEARSON.

The Gables, East Ilsley, Berks.

Applications include:

- dispersion of mosquitoes
- random migration of micro-organisms
- phenomenon of laser speckle

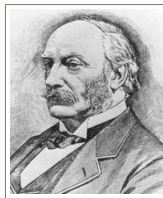
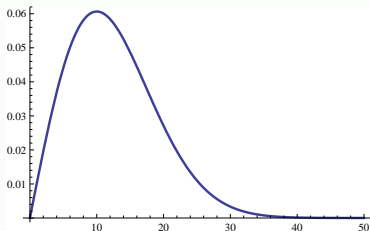
Long random walks



THM
Rayleigh,
1905

$$p_n(x) \approx \frac{2x}{n} e^{-x^2/n} \quad \text{for large } n$$

EG
P200



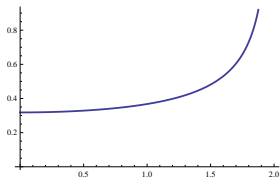
“ The lesson of Lord Rayleigh’s solution is that in open country the most probable place to find a drunken man who is at all capable of keeping on his feet is somewhere near his starting point! ”

Karl Pearson, 1905

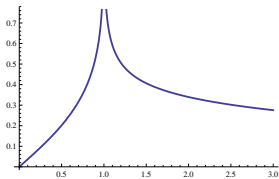


Densities of short walks

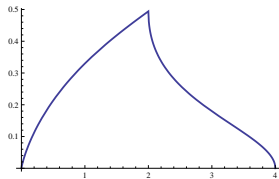
p_2



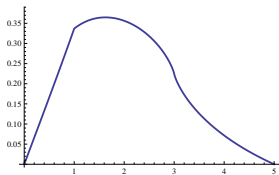
p_3



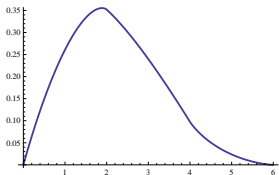
p_4



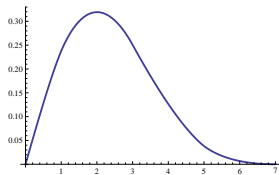
p_5



p_6

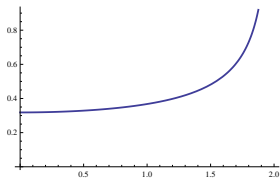


p_7

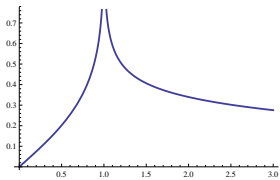


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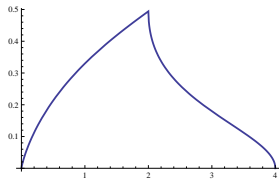
p_2



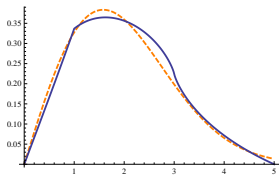
p_3



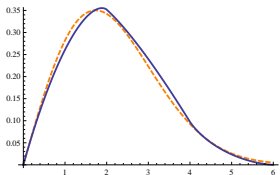
p_4



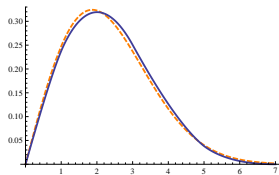
p_5



p_6



p_7



Moments

- The moments of a RV X are $E(X)$, $E(X^2)$, $E(X^3)$, ...
- If X has probability density $f(x)$ then

$$E(X^s) = \int_{-\infty}^{\infty} x^s f(x) dx$$

FACT The moments $E(X^s)$ are analytic in s . (if, e.g., $f(x)$ is compactly supported)

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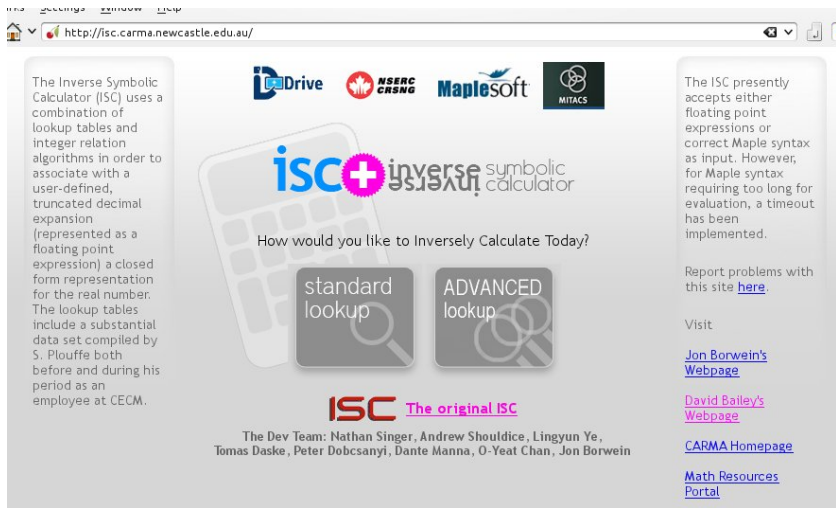
- Represent the k th step by the complex number $e^{2\pi i x_k}$.
- The s th moment of the distance after n steps is:

$$W_n(s) := \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi i x_k i} \right|^s d\mathbf{x}$$

In particular, $W_n(1)$ is the average distance after n steps.

Average distance traveled in two steps

- Numerically: $W_2(1) \approx 1.2732395447351626862$



The Inverse Symbolic Calculator (ISC) uses a combination of lookup tables and integer relation algorithms in order to associate with a user-defined, truncated decimal expansion (represented as a floating point expression) a closed form representation for the real number. The lookup tables include a substantial data set compiled by S. Plouffe both before and during his period as an employee at CECM.

Logos for iDrive, NSERC CRNSG, Maplesoft, and MITACS are displayed at the top.

The main heading reads "isc + inverse symbolic calculator". Below it, the text asks "How would you like to Inversely Calculate Today?" and offers two options: "standard lookup" and "ADVANCED lookup".

The ISC logo is followed by the text "The original ISC". Below this, the Dev Team is listed: "The Dev Team: Nathan Singer, Andrew Shouldice, Lingyun Ye, Tomas Daske, Peter Dobcsanyi, Dante Manna, O-Yeat Chan, Jon Borwein".

On the right side, a text box states: "The ISC presently accepts either floating point expressions or correct Maple syntax as input. However, for Maple syntax requiring too long for evaluation, a timeout has been implemented." Below this, it says "Report problems with this site [here](#)." and "Visit [Jon Borwein's Webpage](#)", "[David Bailey's Webpage](#)", "[CARMA Homepage](#)", and "[Math Resources Portal](#)".

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Logos for iDrive, NSERC CRNSG, MapleSoft, and MITACS are displayed at the top.

The central graphic features a calculator with the text "isc + inverse symbolic calculator" overlaid.

The input field contains the value: 1.2732395447351626862

The "Inverse Calculate" button is highlighted.

Text on the right side: "The ISC presently accepts either floating point expressions or correct Maple syntax as input. However, for Maple syntax requiring too long for evaluation, a timeout has been implemented."

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Text at the bottom: "Here are a few fun numbers to try:"

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Standard inverse calculate found nothing.

[Try Advanced Calculate](#)

ISC The original ISC

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Advanced lookup results for **1.2732395447351626862**

Transform ($K=1.2732395447351626862$)	Searched for	Description
$K^{5/6}$	1.0610329539459689052	$-1/3/\pi$ $2/3/\text{GAM}(1/6)/\text{GAM}(5/6)$ $1/3/\pi$
$K^{3/4}$	954929658561372014653	$3/\pi$
$K^{5/8}$	79577471545947667888	$1/2/\text{GAM}(1/6)/\text{GAM}(5/6)$ $\cos(\pi/12)/\pi \cdot \sin(\pi/12)$ $1/4/\text{sr}(\pi)^2$
$K^{5/9}$	70735530263064593678	$2/9/\pi$
$K^{1/2}$	63661977236758134310	$2/\pi$
$K^{5/12}$	53051647697298445258	$-1/6/\pi$
$K^{3/8}$	47746482927568600732	$3/2/\pi$ $\text{sr}(3)/\text{GAM}(1/3)/\text{GAM}(2/3)$ $3/2/\pi$

The simple two-step case confirmed

- The average distance in two steps:

$$W_2(1) = \int_0^1 \int_0^1 |e^{2\pi i x} + e^{2\pi i y}| \, dx dy = ?$$

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Better: Mathematica 8 and 9 just don't evaluate the double integral.

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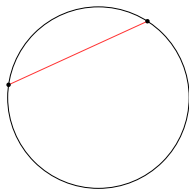
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- This is the average length of a random arc on a unit circle.



Moments of random walks

DEF The s th moment $W_n(s)$ of the density p_n :

$$W_n(s) := \int_0^\infty x^s p_n(x) dx = \int_{[0,1]^n} |e^{2\pi i x_1} + \dots + e^{2\pi i x_n}|^s d\mathbf{x}$$

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- On a desktop:

$$W_3(1) \approx 1.57459723755189365749$$

$$W_4(1) \approx 1.79909248$$

$$W_5(1) \approx 2.00816$$

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Lawrence Berkeley National Laboratory, 256 cores

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- Hard to evaluate numerically to high precision.

Monte-Carlo integration gives approximations with an asymptotic error of $O(1/\sqrt{N})$ where N is the number of sample points.

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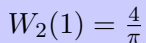
n	$s = 1$	$s = 2$	$s = 3$	$s = 4$	$s = 5$	$s = 6$	$s = 7$
2	1.273	2.000	3.395	6.000	10.87	20.00	37.25
3	1.575	3.000	6.452	15.00	36.71	93.00	241.5
4	1.799	4.000	10.12	28.00	82.65	256.0	822.3
5	2.008	5.000	14.29	45.00	152.3	545.0	2037.
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$$W_3(1) = 1.57459723755189\dots = ?$$

For instance, the sequence $W_3(2k)$ is 1, 3, 15, 93, 639, 4653, ...

The integer sequence database

This site is supported by donations to [The OEIS Foundation](#).

[Hints](#)

(Greetings from [The On-Line Encyclopedia of Integer Sequences!](#))

Search: **seq:1,3,15,93**

Displaying 1-8 of 8 results found.

page 1

Sort: relevance | [references](#) | [number](#) | [modified](#) | [created](#) Format: long | [short](#) | [data](#)

[A002893](#) $\sum_{k=0..n} \text{binomial}(n,k)^2 * \text{binomial}(2k,k)$ +20
(Formerly M2998 N1214) 21

1, 3, 15, 93, 639, 4653, 35169, 272835, 2157759, 17319837, 140668065, 1153462995, 9533639025,
79326566595, 663835030335, 5582724468093, 47152425626559, 399769750195965, 3400775573443089,
29016970072920387, 248256043372999089 ([list](#); [graph](#); [refs](#); [listen](#); [history](#); [text](#); [internal format](#))

OFFSET 0,2

COMMENTS Comment from Matthijs Coster, Apr 28 2004: This is the Taylor expansion of a special point on a curve described by Beauville.

a(n) is the (2n)th moment of the distance from the origin of a 3-step random walk in the plane - Peter M. W. Gill (peter.gill(AT)nott.ac.uk), Feb 27 2004

a(n) is the number of Abelian squares of length 2n over a 3-letter alphabet. [From [Jeffrey Shallit](#), Aug 17 2010]

Consider 2D simple random walk on honeycomb lattice. a(n) gives number of paths of length 2n ending at origin - [Sergey Perepechko](#) Feb 16 2011

Row sums of the square of [A008459](#). - [Peter Bala](#), Mar 05 2013

Conjecture: For each $n=1,2,3,\dots$ the polynomial $g_n(x) = \sum_{k=0}^n \text{binomial}(n,k)^2 * \text{binomial}(2k,k) * x^k$ is irreducible over the field of rational numbers. [[Zhi-Wei Sun](#), Mar 21 2013]

REFERENCES David H. Bailey, Jonathan M. Borwein, David Broadhurst and M. L. Glasser, Elliptic integral evaluations of Bessel moments, arXiv:0801.0891.

P. Barrucand, A combinatorial identity, Problem 75-4, SIAM Rev., 17 (1975), 168.

The integer sequence database

This site is supported by donations to [The OEIS Foundation](#).

[Hints](#)

(Greetings from [The On-Line Encyclopedia of Integer Sequences!](#))

Search: **seq:1,5,45,545**

Displaying 1-1 of 1 result found.

page 1

Sort: [relevance](#) | [references](#) | [number](#) | [modified](#) | [created](#) Format: [long](#) | [short](#) | [data](#)

[A169714](#) The function $W_5(2n)$ (see Borwein et al. reference for definition). +20
5

1, 5, 45, 545, 7885, 127905, 2241225, 41467725, 798562125, 15855173825, 322466645545, 6687295253325, 140927922498025, 3010302779775725, 65046639827565525, 1419565970145097545, 31249959913055650125, 693192670456484513025 ([list](#); [graph](#); [refs](#); [listen](#); [history](#); [text](#); [internal format](#))

OFFSET 0, 2

COMMENTS Row sums of the fourth power of [A008459](#). - [Peter Bala](#), Mar 05 2013

REFERENCES Armin Straub, Arithmetic aspects of random walks and methods in definite integration, Ph. D. Dissertation, School Of Science And Engineering, Tulane University, 2012. - From [N. J. A. Sloane](#), Dec 16 2012

LINKS [Table of \$n, a\(n\)\$ for \$n=0..17\$](#) .
Jonathan M. Borwein, Dirk Nuyens, Armin Straub and James Wan, [Random Walk Integrals](#), 2010.
Jonathan M. Borwein and Armin Straub, [Mahler measures, short walks and log-sine integrals](#) (2012)

FORMULA $\text{Sum}_{\{n \geq 0\}} a(n) \cdot x^n / n!^2 = (\text{Sum}_{\{n \geq 0\}} x^n / n!^2)^5 = \text{BesselI}(0, 2 \cdot \sqrt{x})^5$. - [Peter Bala](#), Mar 05 2013

MAPLE [A169714](#) := proc(n)
 W(5, 2^n) ;
 end proc: # with W() from [A169715](#), [R. J. Mathar](#), Mar 27 2012

CROSSREFS Cf. [A002893](#), [A002895](#), [A169715](#).

- Based on the observation that

$$W_3(2k) = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j},$$

knowledge of **modular forms** allows us to deduce:

THM
Borwein-
Nuyens-
S-Wan,
2010

$$\begin{aligned} W_3(1) &= \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right) \\ &= 1.57459723755189\dots \end{aligned}$$

Modular forms

“ Modular forms are functions on the complex plane that are inordinately symmetric. They satisfy so many internal symmetries that their mere existence seem like accidents. But they do exist. ”
Barry Mazur (BBC Interview, “The Proof”, 1997)

DEF Actions of $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z})$:

- on $\tau \in \mathcal{H}$ by $\gamma \cdot \tau = \frac{a\tau + b}{c\tau + d}$,
- on $f : \mathcal{H} \rightarrow \mathbb{C}$ by $(f|_k\gamma)(\tau) = (c\tau + d)^{-k} f(\gamma \cdot \tau)$.

EG $\mathrm{SL}_2(\mathbb{Z})$ is generated by $T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ and $S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

$$T \cdot \tau = \tau + 1, \quad S \cdot \tau = -\frac{1}{\tau}$$



There's a saying attributed to Eichler that there are five fundamental operations of arithmetic: addition, subtraction, multiplication, division, and modular forms.

Andrew Wiles (BBC Interview, "The Proof", 1997)

DEF A function $f : \mathbb{H} \rightarrow \mathbb{C}$ is a **modular form** of weight k if

- $f|_k \gamma = f$ for all $\gamma \in \mathrm{SL}_2(\mathbb{Z})$,
- f is holomorphic (including at the cusp $i\infty$).

EG

$$f(\tau + 1) = f(\tau), \quad \tau^{-k} f(-1/\tau) = f(\tau).$$

- Similarly, MFs w.r.t. finite-index $\Gamma \leq \mathrm{SL}_2(\mathbb{Z})$
- Spaces of MFs finite dimensional, Hecke operators, ...

- The **Dedekind eta function**

$$(q = e^{2\pi i\tau})$$

$$\eta(\tau) = q^{1/24} \prod_{n \geq 1} (1 - q^n)$$

transforms as

$$\eta(\tau + 1) = e^{\pi i/12} \eta(\tau), \quad \eta(-1/\tau) = \sqrt{-i\tau} \eta(\tau).$$

EG $\Delta(\tau) = (2\pi)^{12} \eta(\tau)^{24}$ is a modular form of weight 12.

Modularity of the three-step moments

- The even moments

1, 3, 15, 93, 639, ...

$$W_3(2k) = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j}$$

have the **modular parametrization**

$$\underbrace{\frac{\eta^6(2\tau)\eta(3\tau)}{\eta^3(\tau)\eta^2(6\tau)}}_{\text{modular form}} = \sum_{k \geq 0} W_3(2k) \underbrace{\left(\frac{\eta(\tau)\eta^2(6\tau)}{\eta^2(2\tau)\eta(3\tau)} \right)^{4k}}_{\text{modular function}} .$$

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EG The values of modular functions at quadratic irrationalities $\tau \in \mathbb{Q}(\sqrt{-d})$ are algebraic!

PSLQ predicts that for the above modular function $x(\tau)$, the value $x(i/3) \approx 0.52754$ has minimal polynomial $1 - 6x^4 - 24x^6 - 3x^8$.

- How does the ISC recognize numbers?

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- **PSLQ** takes numbers $\mathbf{x} = (x_1, x_2, \dots, x_n)$ and tries to find integers $\mathbf{m} = (m_1, m_2, \dots, m_n)$, not all zero, such that

$$\mathbf{x} \cdot \mathbf{m} = m_1 x_1 + \dots + m_n x_n = 0.$$

The vector \mathbf{m} is called an **integer relation** for \mathbf{x} .

In case that no relation is found, PSLQ provides a lower bound for the norm of any potential integer relation.

Integer relation algorithms

- How does the ISC recognize numbers?
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In case that no relation is found, PSLQ provides a lower bound for the norm of any potential integer relation.

EG Is $x = 0.31783724519578224473 \dots$ algebraic?

In[1]:= **PSLQ**[{1, x, x², x³, x⁴}]

Out[1]= {1, 0, -10, 0, 1}

That is, x likely has minimal polynomial $1 - 10x^2 + x^4$.

Therefore, $x = \sqrt{3} - \sqrt{2}$.

- A well-known fact: $\sin((2n - 1)x)$ is a linear combination of $\sin(x), \sin^3(x), \dots, \sin^{2n-1}(x)$

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EG

```
In[1]:= With[{x = 1}, PSLQ[  
          N[{Sin[5x], Sin[x], Sin[x]^3, Sin[x]^5}, 20]]]
```

```
Out[1]= {-1, 5, -20, 16}
```

In other words,

$$\sin(5x) = 5 \sin(x) - 20 \sin^3(x) + 16 \sin^5(x).$$

EG Arithmetic mean \geq geometric mean

In[1]:= **CylindricalDecomposition**[($a+b$)/2 \geq Sqrt[ab], { a, b }]

Out[1]= $a \geq 0 \wedge b \geq 0$

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EG If the sum of four positive numbers is $4c$ and the sum of their squares is $8c^2$, then none of the numbers can exceed $(1 + \sqrt{3})c$.

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EG If the sum of four positive numbers is $4c$ and the sum of their squares is $8c^2$, then none of the numbers can exceed $(1 + \sqrt{3})c$.

In[2]:= **CylindricalDecomposition**[Exists[{ a_2, a_3, a_4 },

$$a_1 \geq a_2 \geq a_3 \geq a_4 > 0 \wedge$$

$$a_1 + a_2 + a_3 + a_4 == 4c \wedge$$

$$a_1^2 + a_2^2 + a_3^2 + a_4^2 == 8c^2], \{c, a_1\}]$$

Out[2]= $c > 0 \wedge 2c < a_1 \leq (1 + \sqrt{3})c$

Positivity of rational functions

- A rational function

$$F(x_1, \dots, x_d) = \sum_{n_1, \dots, n_d \geq 0} a_{n_1, \dots, n_d} x_1^{n_1} \cdots x_d^{n_d}$$

is **positive** if $a_{n_1, \dots, n_d} > 0$ for all indices.

Positivity of rational functions

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EG An obviously positive rational function:

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THM

$$\frac{1}{1 - x - y + \lambda xy}$$

is positive if and only if $\lambda \leq 1$.

Positivity of rational functions

- A rational function

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is **positive** if $a_{n_1, \dots, n_d} > 0$ for all indices.

EG An obviously positive rational function:

$$\frac{1}{1 - x - y + xy} = \frac{1}{(1 - x)(1 - y)}$$

CONJ The following rational function is positive:

Askey–
Gasper
1972

$$\frac{1}{1 - (x + y + z + w) + \frac{2}{3}(xy + xz + xw + yz + yw + zw)}$$

This is a rescaled version of $1/e_2(1 - x, 1 - y, 1 - z, 1 - w)$.

Positivity of rational functions

EG The Askey–Gasper rational function $A(x, y, z)$ and the Szegő rational function $S(x, y, z)$ are positive.

$$A(x, y, z) = \frac{1}{1 - (x + y + z) + 4xyz}$$

$$S(x, y, z) = \frac{1}{1 - (x + y + z) + \frac{3}{4}(xy + yz + zx)}$$

THM
S 2007

There is a **positivity-preserving** operator T such that $T \cdot A = S$.

Positivity of rational functions

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THM
S 2007

There is a **positivity-preserving** operator T such that $T \cdot A = S$.

EG The diagonal Taylor terms of A are given by

$$[x^n y^n z^n] A(x, y, z) = \sum_{k=0}^n \binom{n}{k}^3.$$

By **WZ**, both sides satisfy the recurrence

$$(n+1)^2 a_{n+1} = (7n^2 + 7n + 2)a_n + 8n^2 a_{n-1}.$$

EG The diagonal Taylor terms of $S(2x, 2y, 2z)$, namely

1, 12, 198, 3720, 75690, 1626912, \dots ,

satisfy the recurrence

$$2(n+1)^2 s_{n+1} = 3(27n^2 + 27n + 8) s_n - 81(3n-1)(3n+1) s_{n-1}.$$

Positivity of rational functions

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To prove positivity from the recurrence, apply CAD to the formula

$$(\forall n, A, B) \quad n \geq 1, A \geq 0, B \geq \lambda A \implies C \geq \lambda B$$

$$\text{where } 2(n+1)^2 C = 3(27n^2 + 27n + 8)B - 81(3n-1)(3n+1)A.$$

Positivity of rational functions

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```
In[1]:= With[{C = ...},  
  CylindricalDecomposition[ForAll[{n, A, B},  
    n >= 1 & B >= lambda A & A >= 0, C >= lambda B], {lambda}]]
```

```
Out[1]= 27/2 <= lambda <= 3/8(31 + sqrt(385))
```

Positivity of rational functions

- The Kauers–Zeilberger rational function

$$\frac{1}{1 - (x + y + z + w) + 2(yzw + xzw + xyw + xyz) + 4xyzw}$$

is conjectured to be positive.

- Its positivity implies the positivity of the Askey–Gasper function

$$\frac{1}{1 - (x + y + z + w) + \frac{2}{3}(xy + xz + xw + yz + yw + zw)}.$$

PROP
S-Zudilin
2013

The Kauers–Zeilberger function has diagonal coefficients

$$d_n = \sum_{k=0}^n \binom{n}{k}^2 \binom{2k}{n}^2.$$

Q Under what condition(s) is the positivity of a rational function

$$h(x_1, \dots, x_d) = \frac{1}{\sum_{k=0}^d c_k e_k(x_1, \dots, x_d)}$$

implied by the positivity of its diagonal?

- Is the positivity of $h(x_1, \dots, x_{d-1}, 0)$ a sufficient condition?

EG $\frac{1}{1+x+y}$ has positive diagonal coefficients but is not positive.

Positivity of rational functions

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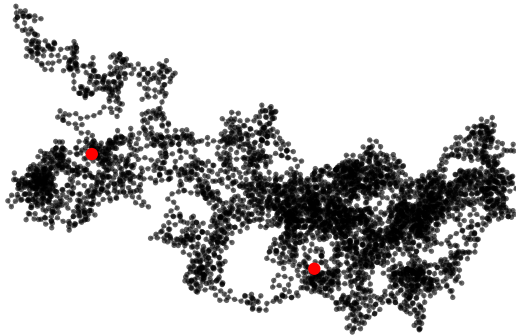
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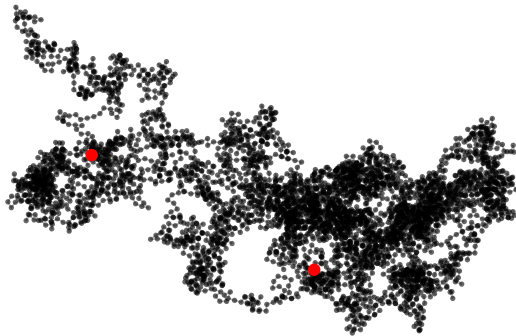
$$h(x, y) = \frac{1}{1 + c_1(x + y) + c_2xy}$$

is positive iff $h(x, 0)$ and the diagonal of $h(x, y)$ are positive.

Drunken birds



Drunken birds



“ *A drunk man will find his way home,
but a drunk bird may get lost forever.* ”
Shizuo Kakutani, 1911–2004



THANK YOU!

Slides for this talk will be available from my website:
<http://arminstraub.com/talks>



A. Straub, W. Zudilin

Positivity of rational functions and their diagonals

Preprint, 2013



J. Borwein, A. Straub, J. Wan, W. Zudilin (appendix by D. Zagier)

Densities of short uniform random walks

Canadian Journal of Mathematics, Vol. 64, Nr. 5, 2012, p. 961-990



J. Borwein, D. Nuyens, A. Straub, J. Wan

Some arithmetic properties of short random walk integrals

The Ramanujan Journal, Vol. 26, Nr. 1, 2011, p. 109-132



A. Straub

Positivity of Szegő's rational function

Advances in Applied Mathematics, Vol. 41, Issue 2, Aug 2008, p. 255-264