Walks in Cones and Tight Enclosures of Laplacian Eigenvalues

Bruno Salvy

AriC, Inria, ENS de Lyon

20

15

012345678



Joint work with Joel Dahne



SIAM J. Sci. Comp. 2020 doi: 10.1137/20M1326520 arXiv: abs/2003.08095 I. Long Introduction: Walks in Cones

Lattice Walks: a Mine of Linear **Recurrences Waiting for Tools** 20 Walks from 0 to $P \in \mathbb{Z}^d$ staying in $K \subset \mathbb{R}^d$ using *n* steps in $\mathcal{S} \subset \mathbb{Z}^d$ 15 **Ex.:** $d = 2, \ \mathcal{S} = \{\uparrow, \downarrow, \rightarrow, \leftarrow, \diagdown\}, \ K = \mathbb{N}^2$ $u_{i,j,n} = u_{i-1,j,n-1} + u_{i,j-1,n-1} + u_{i+1,j,n-1} + u_{i,j+1,n-1} + u_{i+1,j+1,n-1}$ $u_{i,i,n} = 0$ for $(i,j) \notin K$ Generating functions: excursions total number $U_{K}(x,y;z) := \sum u_{i,j,n} x^{i} y^{j} z^{n}, \quad U_{K}(0,0;z) = \sum e_{n} z^{n}, \quad U_{K}(1,1;z) = \sum u_{n} z^{n}.$ i,j,nApplications: queuing theory, statistical physics, combinatorics,...

Questions: $S, K \rightarrow$ asymptotics? nature of these series?



$U_{\mathbb{N}^2}(x, y; z)$ is algebraic

[Kreweras65, Niederhausen83, Gessel86, BousquetMelou05, Bernardi07, BernardiBousquet-MélouRaschel21]

Main Character: Generating Polynomial

$$\chi_{\mathcal{S}}(x_{1},...,x_{d}) := \sum_{s \in \mathcal{S}} x_{1}^{s_{1}} \cdots x_{d}^{s_{d}}$$
For $k \in \mathbb{N}$, $\chi_{\mathcal{S}}^{k} = \sum_{m \in \mathbb{Z}^{d}} c_{k,m} x_{1}^{m_{1}} \cdots x_{d}^{m_{d}}$
num. walks from 0
to *m* in \mathbb{Z}^{d} in *k* steps
Summing over k , $\frac{1}{1 - z\chi_{\mathcal{S}}} = \sum_{k,m} c_{k,m} x^{m} z^{k} = U_{\mathbb{Z}^{d}}(x; z)$
For an arbitrary cone *K*,

Kernel equation

 $(1 - z\chi_S)U_K(x; z) = 1 + \text{correcting terms encoding } \partial K$

A Mysterious Secondary Character: Group of the Walk

For *small-step* walks $(\max_i |s_i| = 1, \text{ for all } s \in \mathcal{S})$

For all $i \in \{1, ..., d\}$, $\chi_{\mathcal{S}} = A_i^- x_i^{-1} + A_i^0 + A_i^+ x_i$,

 $A_i^-, A_i^0, A_i^+ \in \mathbb{Z}[x_1^{\pm 1}, \dots, x_{i-1}^{\pm 1}, x_{i+1}^{\pm 1}, \dots, x_d^{\pm 1}]$

$$\psi_i : \left(x_j \mapsto x_j \text{ for } j \neq i, x_i \mapsto \frac{A_i^- 1}{A_i^+ x_i} \right) \text{ fixes } \chi_{\mathscr{S}}$$

Group: $\mathscr{G}_{\mathcal{S}} := \langle \psi_1, ..., \psi_d \rangle$ generated by the ψ_i .

[Malyshev, Fayolle, Iasnogordski, Mishna, Bousquet-Mélou]

D Springer

Random

Walks in the

Juarter Plane

Classes of Univariate Power Series



Knowing where U(z) fits helps deduce properties of (u_n) .

Generating Functions and Asymptotics

For
$$U(z) := \sum_{n=0}^{\infty} u_n z^n \in \mathbb{Q}[[z]]$$

if $u_n \sim C \rho^n n^{\alpha}$, $n \to \infty$



Conversely, asymptotics help classify.

Walks in \mathbb{N}^2 : Recent Progress



[Bernardi,Bostan,Bousquet-Mélou,Gessel,Gouyou-Beauchamps,Hardouin,Kauers, Kreweras,Melczer,Mishna,Raschel,Rechnitzer,Roques,Salvy,Singer]



Asymptotics: $e_n \sim C 5^n n^{\alpha}$ with $\alpha = -1 - \frac{\pi}{\arccos(1/4)}$ Next 2 slides

 $\alpha \notin \mathbb{Q}$ $\Rightarrow U(0,0,z) \text{ not D-finite}$ $\Rightarrow U(x, y, z) \text{ not D-finite}$ Proof: $\alpha \in \mathbb{Q}$ $\Rightarrow z \text{ root of unity, with}$ $\frac{z+1/z}{2} = \frac{1}{4}$ $\Rightarrow 2z^2 - z + 2 \text{ divisible by a cyclotomic pol.}$ Contradiction.

[BostanRaschelSalvy2014]

Asymptotics from Probabilities (1/2)

Hyp.

$$\mathcal{S} := \{s_1, \dots, s_N\} \subset \mathbb{Z}^d$$

K a cone with apex at 0

No drift:
$$\sum_{i} s_{i} = 0$$

Normalized: $\left(\sum_{k=1}^{d} s_{i}^{(k)} s_{j}^{(k)}\right)_{i,j} = \mathbf{Id}$

+ non-degeneracy conditions

+ regularity conditions on ∂K

def soon

Conclusion

#excursions ~
$$C | \mathcal{S} |^n n^{-\alpha_{\mathcal{S}}}$$
,



$$\alpha_{\mathcal{S}} := \sqrt{\lambda_1 + (d/2 - 1)^2 + 1},$$

 λ_1 : tundamental eigenvalue of $\Delta_{\mathbb{S}^{d-1}}$ on $\mathbb{S}^{d-1} \cap K$

Principle: reduce to Brownian motion in *K*

[DenisovWachtel2015]



Asymptotics from Probabilities (2/2)

- Reduce cases with drifts and covariance by
- 1. Adding weights $1/w_i$, w_i to the steps in direction i, for i = 1, ..., d
- 2. A linear change *M* of coordinates

Conclusion

Partial combinatorial explanation for ρ #excursions ~ $C \rho^n n^{-\alpha_s}$, $\rho := |\mathcal{S}| \min_{(x_1, \dots, x_d) \in \mathbb{R}^d_+} \chi(x_1, \dots, x_d)$ $\alpha := \sqrt{\lambda_1 + (d/2 - 1)^2 + 1},$ λ_1 : fundamental eigenvalue of $\Delta_{\mathbb{S}^{d-1}}$ on $\mathbb{S}^{d-1} \cap MK$.

[DenisovWachtel15, JohnsonMishnaYeats18]

Example: Kreweras 3D

The group of the walk is finite



Excursions: $e_n \sim C 4^n n^{-\alpha_{\kappa}}$



Previous estimates lead to:

 $\begin{array}{ll} \alpha_{\kappa} \in [3.323, 3.326] & (Costabel, 2008) \\ \alpha_{\kappa} \simeq 3.32572 & (Ratzkin, Treibergs, 2009) \\ \alpha_{\kappa} \simeq 3.3261 & (Balakrishna, 2013) \\ \alpha_{\kappa} \simeq 3.325757004174456 & (Guttmann, 2015) \\ \alpha_{\kappa} \simeq 3.3257569 & (Bacher et al., 2016) \\ \alpha_{\kappa} \simeq 3.325757004175 & (Bogosel et al., 2020) \end{array}$

Initial goal of this work

New: If
$$\alpha_{\kappa} = p/q \in \mathbb{Q}$$
, then $q > 10^{51}$.

D-finiteness more and more doubtful

Walk-mining in \mathbb{N}^3

(Bogosel, Perrollaz, Raschel, Trotignon 2020)

17 spherical triangles associated to finite groups

- + computation of the corresponding angles (all in $\{\pi/4, \pi/3, \pi/2, 2\pi/3, 3\pi/4\}$)
- + exact or estimated value of the exponent



They all correspond to tilings of the sphere

Results

Angles	BPRT	new
$(3\pi/4,\pi/3,\pi/2)$	12.400051	$12.400051652843377905 \pm 10^{-47}$
$(2\pi/3,\pi/3,\pi/2)$	13.744355	$13.744355213213231835 \pm 10^{-84}$
$(2\pi/3,\pi/4,\pi/2)$	20.571973	$20.571973537984730557 \pm 10^{-30}$
$(2\pi/3,\pi/3,\pi/3)$	21.309407	$21.309407630190445260 \pm 10^{-206}$
$(3\pi/4,\pi/4,\pi/3)$	24.456913	$24.456913796299111694 \pm 10^{-73}$
$(2\pi/3,\pi/4,\pi/4)$	49.109945	$49.109945263284609920 \pm 10^{-153}$
$(2\pi/3, 3\pi/4, 3\pi/4)$	4.261734	$4.2617347552939870857 \pm 10^{-22}$
$(2\pi/3, 2\pi/3, 2\pi/3)$	5.159145	$5.1591456424665417112 \pm 10^{-104}$
$(\pi/2, 2\pi/3, 3\pi/4)$	6.241748	$6.2417483307263342368 \pm 10^{-20}$
$(\pi/2, 2\pi/3, 2\pi/3)$	6.777108	$6.7771080545983009573 \pm 10^{-35}$
olomonts &)	

finite elements & convergence acceleration

[BogoselPerrollazRaschelTrotignon20]

Next: How do we do it? and why are the precisions so different? 13/32

II. Laplacian on Spherical Triangles

Fundamental Eigenvalue of the Laplace-Beltrami Operator on the Unit Sphere

Laplace operator in spherical coordinates in \mathbb{R}^d

$$\Delta f = r^{1-d} \frac{\partial}{\partial r} \left(r^{d-1} \frac{\partial f}{\partial r} \right) + r^{-2} \Delta_{\mathbb{S}^{d-1}} f$$
Laplace-Beltrami on the sphere
Eigenvalue problem for $\Omega \subset \mathbb{S}^{d-1}$:
 $\Delta_{\mathbb{S}^{d-1}} f + \lambda f = 0$ in Ω , $f|_{\partial\Omega} = 0$.
Dirichlet condition
Goal: $(\alpha, \beta, \gamma) \mapsto \lambda_1$ with high precision
(dimension $d=3$)

Basic Properties of the Laplacian over a Hold also for $\Delta_{\mathbb{S}^{d-1}}$ Bounded Domain $\Omega \subset \mathbb{R}^d$

- . self-adjoint: $(\Delta u, v) = (u, \Delta v)$ on $\{f \in C^2(\Omega), f|_{\partial\Omega} = 0\}$. discrete spectrum with no accumulation point
- fundamental eigenvalue $0 < \lambda_1 < \lambda_2 \leq \cdots, \quad \lambda_n \to \infty$
 - . corresponding eigenfunctions (u_n) Hilbert basis of $L_2(\Omega)$
 - . maximum principle: $\Delta u \ge 0$ in $\Omega \Rightarrow \sup_{x \in \Omega} u(x) \le \sup_{x \in \partial \Omega} u(x)$
 - . monotonicity: $\Omega \subset \Omega' \Rightarrow \lambda_i(\Omega) \ge \lambda_i(\Omega')$, for all i
 - . Faber-Krahn inequality: $\lambda_1(\Omega) \ge \lambda_1(\Omega^*)$,
 - $\Omega^{\star} = \begin{cases} \text{ball with the same volume for } \Delta, \\ \text{spherical cap with the same area for } \Delta_{\mathbb{S}^{d-1}}. \end{cases}$

Matlab logo

15/32

 $(u, v) := \frac{1}{\operatorname{Vol}\Omega} \left[uv \, d\sigma \right]$

Planar Case



Spherical Triangles

Eigenvalues known when $(\alpha, \beta, \gamma) = \left(\frac{\pi}{p}, \frac{\pi}{q}, \frac{\pi}{r}\right)$ Only possible (p, q, r) that give triangles:

$$\begin{array}{l} (2,3,3) \longrightarrow \lambda = k(k+1), \ k \in 6+3\mathbb{N}+4\mathbb{N} \\ (2,3,4) \longrightarrow \lambda = k(k+1), \ k \in 9+6\mathbb{N} \\ (2,3,5) \longrightarrow \lambda = k(k+1), \ k \in 15+6\mathbb{N}+10\mathbb{N} \\ (2,2,r) \longrightarrow \lambda = k(k+1), \ k \in r+1+2\mathbb{N}+r\mathbb{N} \\ \alpha := \sqrt{\lambda_1 + (d/2-1)^2} + 1 \in \mathbb{Q} \end{array}$$

No other value known —> turn to numerical computation

[Berard1983,BogoselPerrollazRaschelTrotignon18]

17/32

This solves 7

of the 17

finite groups

for 3D walks

Bounds from an Approximate Eigenvalue

Eigenvalue problem for
$$\Omega$$
:
 $\Delta f + \lambda f = 0$ in Ω , $f|_{\partial\Omega} = 0$.
replace by f small
Thm. If $\Delta f^* + \lambda^* f^* = 0$ in Ω , then there exists λ s.t.
 $\frac{|\lambda - \lambda^*|}{\lambda} \leq \frac{\sup_{x \in \partial\Omega} |f^*(x)|}{||f^*||_2}$.

Method:

1. Find a good approximate pair (f^*, λ^*) 2. Compute the bound in a certified way 3. Certify the index

Cost of certification: not large

[FoxHenriciMoler67,MolerPayne68]

$$\frac{|\lambda - \lambda^{\star}|}{\lambda} \leq \frac{\sup_{x \in \partial \Omega} |f^{\star}(x)|}{\|f^{\star}\|_{2}}.$$

Use

$$(u_n) \text{ orthonormal basis, with } \Delta u_n = \lambda_n u_n, \ u_n \big|_{\partial_\Omega} = 0$$

$$w \text{ solution of } \Delta w = 0, \ w \big|_{\partial\Omega} = f^* \big|_{\partial\Omega} \qquad \text{If small, } \|w\| \text{ small}$$
Coefficients of $w: (w, u_n) = (w - f^*, u_n) + (f^*, u_n) = \frac{1}{\lambda_n} (w - f^*, \Delta u_n) + (f^*, u_n),$

$$\Delta \text{ self-adjoint} \qquad = \frac{1}{\lambda_n} (\Delta w - \Delta f^*, u_n) + (f^*, u_n) = \left(1 - \frac{\lambda^*}{\lambda_n}\right) (f^*, u_n).$$
Take λ where $\|(w, u_n)\| \ge \left|1 - \frac{\lambda^*}{\lambda}\right| |(f^*, u_n)|, \qquad \text{discrete spectrum with no accumulation point}$

$$\sum_{\substack{x \in \partial\Omega \\ max. ppl}} \int_{x \in A}^{2} \|f^*\|^2.$$

$$\sum_{\substack{x \in A\Omega \\ max. ppl}} \int_{x \in A}^{2} \|f^*\|^2.$$

Proof

1. Find a good approximate pair $(f^{\star}, \lambda^{\star})$

- 2. Compute the bound in a certified way
- 3. Certify the index

Step 1. Find a good approximate pair (f^*, λ^*)

$$\frac{|\lambda - \lambda^{\star}|}{\lambda} \leq \frac{\sup_{x \in \partial \Omega} |f^{\star}(x)|}{\|f^{\star}\|_{2}}$$

High precision needed, and no guarantee

Method of Particular Solutions

Target:
$$\Delta f^* + \lambda^* f^* = 0$$
 in Ω , $\sup_{x \in \partial \Omega} |f^*|$ small.

1. Fix λ 2. Find a set $(u_{\lambda}^{(k)})_{k=1}^{N}$ of solutions of $\Delta f + \lambda f = 0$ in Ω 3. Find a linear combination $\sum_{k=1}^{N} c_k u_{\lambda}^{(k)}$ that is *k*=1 . small on $\partial \Omega$. not too small on Ω 4. Repeat to minimize sup over λ $x \in \partial \Omega$

20/32

[Bergman47, Vekua48, FoxHenriciMoler67, BetckeTrefethen05, Betcke08]

2. Set of Eigenfunctions



3. Small on
$$\partial \Omega$$
, Not too Small on Ω
 $u_{\lambda}(\phi) := \sum_{k=1}^{N} c_k \sin(\mu_k \phi) \mathsf{P}_{\nu}^{\mu_k}(\cos \theta(\phi))$
with $\lambda = \nu(\nu + 1)$
Satisfies
 $\Delta u_{\lambda} + \lambda u_{\lambda} = 0$
NUME: c_k s.t. $u_{\lambda}|_{[0,\phi_{\max}]} \approx 0$, $||u_{\lambda}||_{\Omega} \approx 1$.
Choose x_1, \dots, x_{m_b} on $\partial \Omega$, y_1, \dots, y_{m_i} inside Ω ;
Form a matrix $A := \begin{pmatrix} u_{\lambda}^{(k)}(x_i) \\ u_{\lambda}^{(k)}(y_i) \end{pmatrix}$
Compute its QR factorization $A = \begin{pmatrix} Q_{\partial \Omega} \\ Q_{\Omega} \end{pmatrix} R$
 $\sigma := \min_{\|\nu\|=1} \|Q_{\partial\Omega}\nu\|$ found together with ν by SVD (least squares)
Recover c by solving $Rc = \nu$.
[BetckeTrefethen05]

22/32

4. Optimize over λ

Ex. Regular Triangle: $(2\pi/3, \pi/3, \pi/2)$



Regular vs Singular Triangles



Def. a corner is regular if its angle is $\pi/k, k \in \mathbb{N}^*$, singular otherwise.

At a regular corner, eigenfunctions can be continued analytically (by reflection).

Expansions from a singular corner converge well is when the other corners are regular, poorly otherwise.

3d-Kreweras is singular

Fix: use a sum of 4 expansions

$$f^{\star}(\theta, \phi) = u_1(\theta_1, \phi_1) + u_2(\theta_2, \phi_2) + u_3(\theta_3, \phi_3) + u_{\text{int}}(\theta_{\text{int}}, \phi_{\text{int}})$$

One from each corner, one from an interior point



1. Find a good approximate pair $(f^{\star}, \lambda^{\star})$

- 2. Compute the bound in a certified way
- 3. Certify the index

Step 2. Rigorous Bounds

$$\frac{|\lambda - \lambda^{\star}|}{\lambda} \leq \frac{\sup_{x \in \partial \Omega} |f^{\star}(x)|}{\|f^{\star}\|_{2}}.$$

Basic Tool: Interval Arithmetic

Replace all floating-point operations by set operations

[1.2, 1.3] + [2.0, 2.1] = [3.2, 3.4] $[1.2, 1.3] \times [2.0, 2.1] = [2.40, 2.73]$

provides certified enclosures

Implementation requires care with rounding modes

We use <u>https://arblib.org/</u>

Weakness: wrapping effect

 $f := e^{-t} - (1 - t + t^2/2! + \dots - t^9/9!)$

f([1.0,1.1]) = [-0.161,0.161] while $f: [1.0,1.1] \mapsto [2.5 \ 10^{-7}, 6.5 \ 10^{-7}]$

Situation very similar to our $f^{\star} = \sum c_k u_{\lambda}^{(k)}$ on $\partial \Omega$



The expensive part of the certification

[MakinoBerz03]

26/32

Lower Bound on the Norm Ζ **Regular Triangles** $\frac{|\lambda - \lambda^{\star}|}{\lambda} \leq \frac{\sup_{x \in \partial \Omega} |f^{\star}(x)|}{\|f^{\star}\|_{2}}$ sine $r d\theta$ dA $r \sin\theta d\phi$ $\int f^{\star} = \sum c_k u_k^{(\lambda)} \qquad u_{\lambda}^{(k)}(\theta, \phi) = \frac{\sin(\mu_k \phi) \mathsf{P}_{\nu}^{\mu_k}(\cos \theta)}{\mathsf{P}_{\nu}^{\mu_k}(\cos \theta)}$ dø Φ $\int_{0}^{\phi_{\max}} \int_{0}^{\theta(\phi)} f^{\star}(\theta,\phi)^{2} \sin\theta \, d\theta \, d\phi \geq \int_{0}^{\phi_{\max}} \int_{0}^{\theta_{\min}} f^{\star}(\theta,\phi)^{2} \sin\theta \, d\theta \, d\phi$ $\geq \frac{\phi_{\max}}{2} \sum c_k^2 \int_{0}^{\theta_{\min}} (\mathsf{P}_{\nu}^{\mu_k}(\cos\theta))^2 \sin\theta \, d\theta$ Orthogonality of $sin(\mu_k \phi)$ **Rigorous** interval evaluation (Arb)

Lower Bound on the Norm



in our computations

[Gómez-SerranoOrriols21]

28/32

Results

Angles	eigenvalue	
$(3\pi/4,\pi/3,\pi/2)$	$12.400051652843377905 \pm 10^{-47}$	
$(2\pi/3,\pi/3,\pi/2)$	$13.744355213213231835 \pm 10^{-84}$	
$(2\pi/3,\pi/4,\pi/2)$	$20.571973537984730557 \pm 10^{-30}$	regular
$(2\pi/3,\pi/3,\pi/3)$	$21.309407630190445260 \pm 10^{-206}$	triangles
$(3\pi/4,\pi/4,\pi/3)$	$24.456913796299111694 \pm 10^{-73}$	
$(2\pi/3,\pi/4,\pi/4)$	$49.109945263284609920 \pm 10^{-153}$	more work
$(2\pi/3, 3\pi/4, 3\pi/4)$	$4.2617347552939870857 \pm 10^{-22}$	for this one singular trianglos
$(2\pi/3, 2\pi/3, 2\pi/3)$	$5.1591456424665417112 \pm 10^{-104}$	
$(\pi/2, 2\pi/3, 3\pi/4)$	$6.2417483307263342368 \pm 10^{-20}$	
$(\pi/2, 2\pi/3, 2\pi/3)$	$6.7771080545983009573 \pm 10^{-35}$	ulangics

1. Find a good approximate pair $(f^{\star}, \lambda^{\star})$

- 2. Compute the bound in a certified way
- 3. Certify the index

Step 3. Certify the index

Certification of the index

monotonicity
$$\lambda < \lambda_2(\Omega') \leq \lambda_2(\Omega)$$
 with $\Omega' \supset \Omega \Rightarrow \lambda = \lambda_1(\Omega)$

For the domain $0 \le \phi \le \phi_{\max}$, $0 \le \theta \le \theta_{\max}$, the eigenvalues are $\nu(\nu + 1)$ with ν root of

 $P_{\nu}^{\mu} \text{ satisfies}$ $((1 - x^2)w')' + q_{\mu,\nu}(x)w = 0,$ $q_{\mu,\nu}(x) = \nu(\nu + 1) - \frac{\mu^2}{1 - x^2}$

$$\mathsf{P}^{\mu_k}_{\nu}(\cos\theta_{\max})=0$$

For each $k \in \mathbb{N}^*$, an infinity of roots $\nu_{k,j}, j \in \mathbb{N}^*$

It is sufficient to check λ against $u_{1,2}$ and $u_{2,1}$

Proof via Sturm's comparison theorem

Sometimes this fails, but another orientation of the triangle works

Bound on Denominator



Last convergent: P/Q with $Q = 95716...26933 > 10^{51}$

If $\alpha_{\kappa} = p/q \in \mathbb{Q}$, then $q > 10^{51}$.

Summary & Conclusion

- Linear recurrences with constant coefficients remain mysterious;
- lattice walks provide a simple source of examples;
- more and more tools are available;
- numerical computation can yield rigorous results, useful in experimental mathematics.

Thank you.