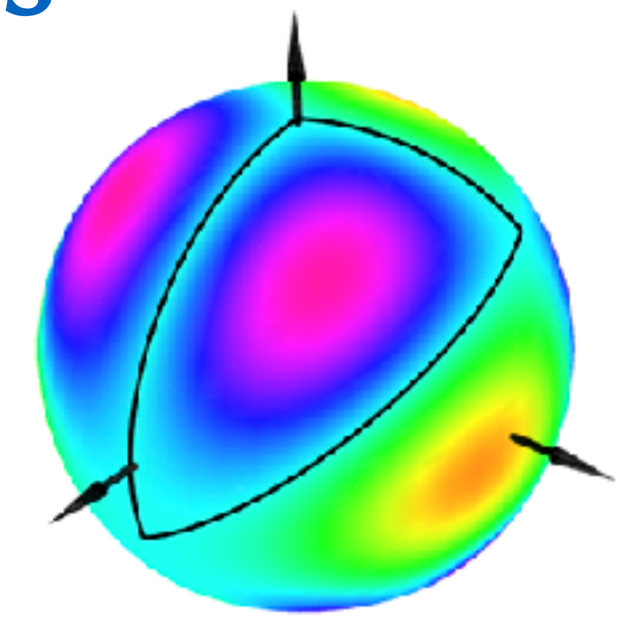
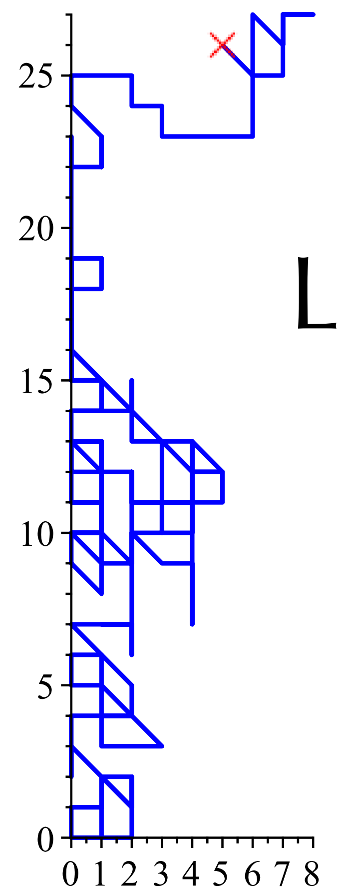
Walks in Cones and Tight Enclosures of Laplacian Eigenvalues



Bruno Salvy

Inria, ENS de Lyon



Lattice Paths, Combinatorics and Interactions

June 2021

Joint work with Joel Dahne

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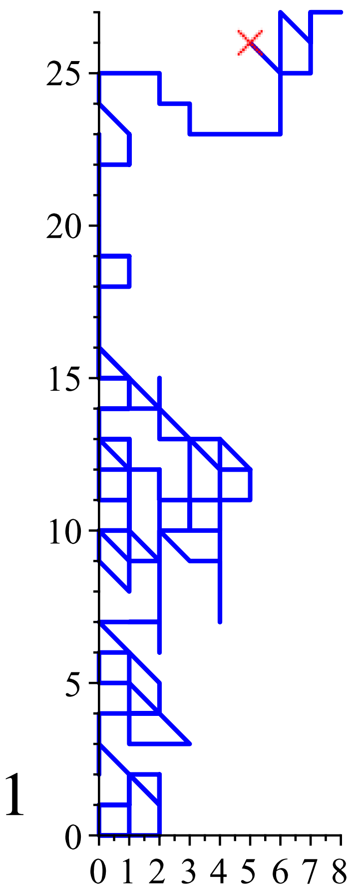
I. Motivation: Walks in Cones

Lattice Walks: a Mine of Linear Recurrences Waiting for Tools



Walks from 0 to $P \in \mathbb{Z}^d$ staying in $K \subset \mathbb{R}^d$
using n steps in $\mathcal{S} \subset \mathbb{Z}^d$

Ex.: $d = 2,\ \mathcal{S} = \{\uparrow, \downarrow, \rightarrow, \leftarrow, \nwarrow\},\ K = \mathbb{N}^2$

$$u_{i,j,n} = u_{i-1,j,n-1} + u_{i,j-1,n-1} + u_{i+1,j,n-1} + u_{i,j+1,n-1} + u_{i+1,j+1,n-1}$$

$$u_{i,j,n} = 0 \quad \text{for} \quad (i,j) \notin K$$

Generating functions:

excursions

total number

$$U_K(x,y;z) := \sum_{i,j,n} u_{i,j,n} x^i y^j z^n, \quad U_K(0,0;z) = \sum_{n\geq 0} e_n z^n, \quad U_K(1,1;z) = \sum_{n\geq 0} u_n z^n.$$

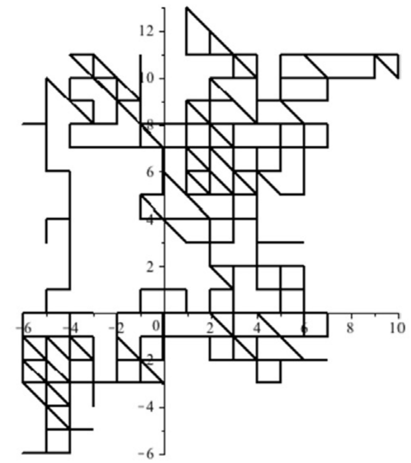
Applications: queuing theory, statistical physics, combinatorics,…

Questions: $\mathcal{S}, K \to$ asymptotics? nature of these series?

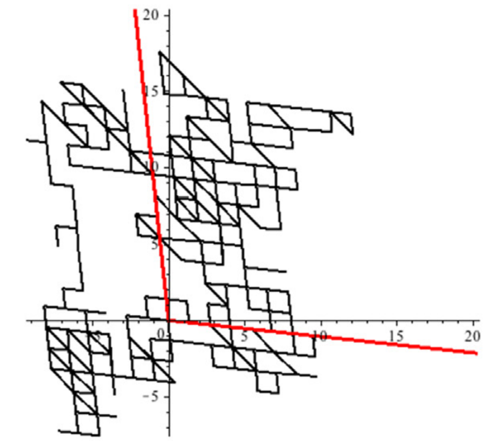
Non-D-Finite Generating Functions of Walks in $\mathbb{N}^d$

$\mathcal{S} = \{\uparrow, \downarrow, \rightarrow, \leftarrow, \searrow\}$

Idea: Normalize so that the asymptotic behaviour is a Brownian motion



a. fix probabilities for each step that remove drift



b. linear transform to remove correlation

$\mathbb{N}^d$ becomes a cone K

Probabilistic ingredient:

$$e_n \sim C\rho^n n^{-p/2} \text{ with } p = \sqrt{\lambda_1 + (d/2-1)^2} - (d/2-1) > 0,$$

λ_1 fundamental eigenvalue of $\Delta_{\mathbb{S}^{d-1}}$ on $\Omega := K \cap \mathbb{S}_{d-1}$.

Def next page

Arithmetic ingredient:

$U(z)$ D-finite, convergent, with integer coefficients $\Rightarrow p \in \mathbb{Q}$.

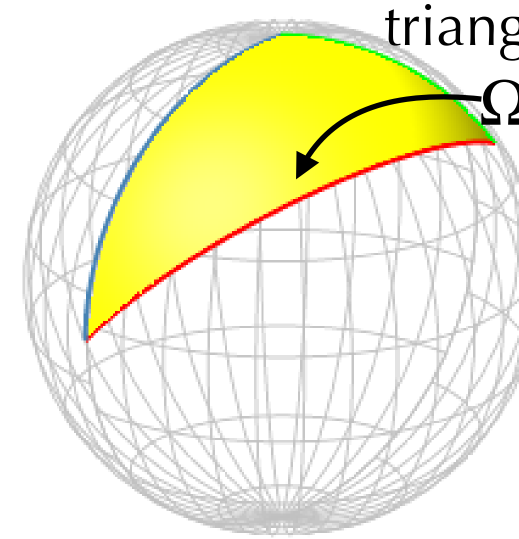
[DenisovWachtel15;Chudnovsky85;André89;Katz70]

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

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

Laplace-Beltrami on the sphere

$$\Delta f = r^{1-d}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial f}{\partial r}\right) + r^{-2}\Delta_{\mathbb{S}^{d-1}} f$$



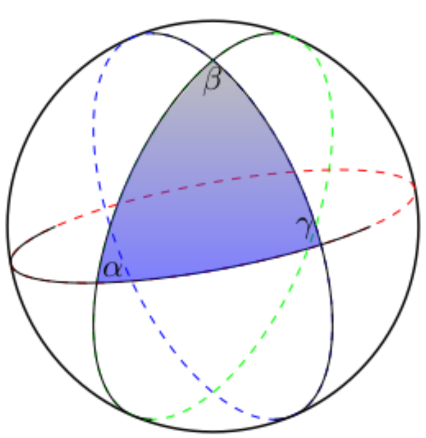
Eigenvalue problem for $\Omega \subset \mathbb{S}^{d-1}$:

$$\Delta_{\mathbb{S}^{d-1}} f + \lambda f = 0 \text{ in } \Omega, \quad f|_{\partial\Omega} = 0.$$

Dirichlet condition

Classical fact: $0 < \lambda_1 < \lambda_2 \leq \cdots, \quad \lambda_n \to \infty$

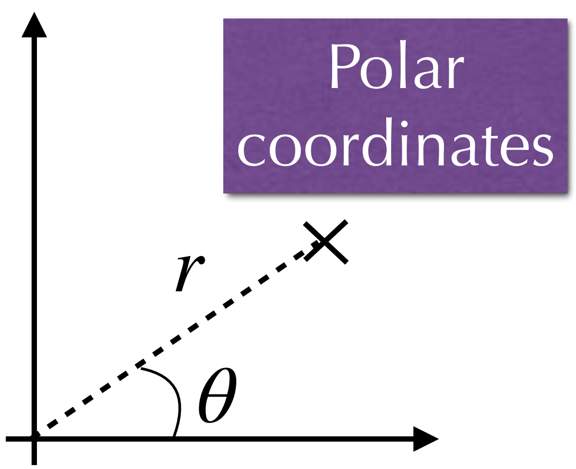
dominant eigenvalue



Goal: $(\alpha, \beta, \gamma) \mapsto \lambda_1$ with high precision

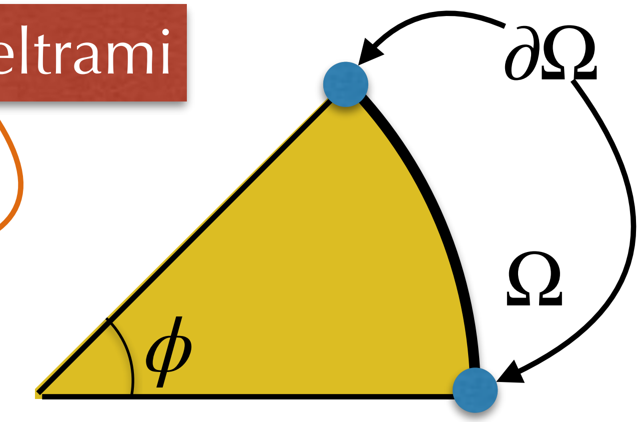
(dimension d=3)

Planar Case

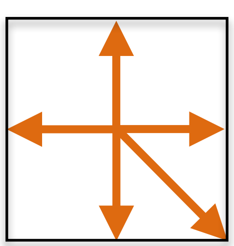


Laplace-Beltrami

$$\Delta f(r,\theta) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2}$$



Eigenfunctions: $\sin(\sqrt{\lambda}\theta + c)$



Boundary: $\begin{cases} \theta = 0 \to c = 0 \\ \theta = \phi \to \lambda = \lambda_k := \left(\dfrac{k\pi}{\phi}\right)^2, k \in \mathbb{N}^\star . \end{cases}$

Ex. $\mathcal{S} = \{\uparrow, \downarrow, \rightarrow, \leftarrow, \searrow\}$, $\phi = \arccos(u)$, $\mu_u(u) = 0$, $\mu_u = 8t^3 - 8t^2 + 6t - 1$

exponent $-\dfrac{p}{2} = 1 + \dfrac{\pi}{\arccos(u)} \notin \mathbb{Q} \Rightarrow$ U not D-finite.

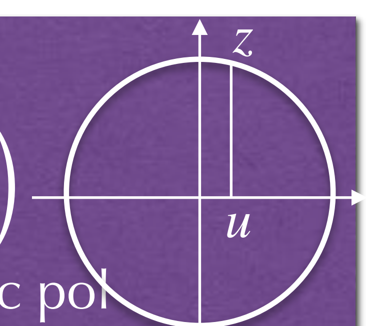
Automatic proof of 51 of the 56 non-Dfinite small-step cases

Proof: $p \in \mathbb{Q}$

$\Rightarrow$ numer $\mu_u\left(\dfrac{z+1/z}{2}\right)$

divisible by a cyclotomic pol

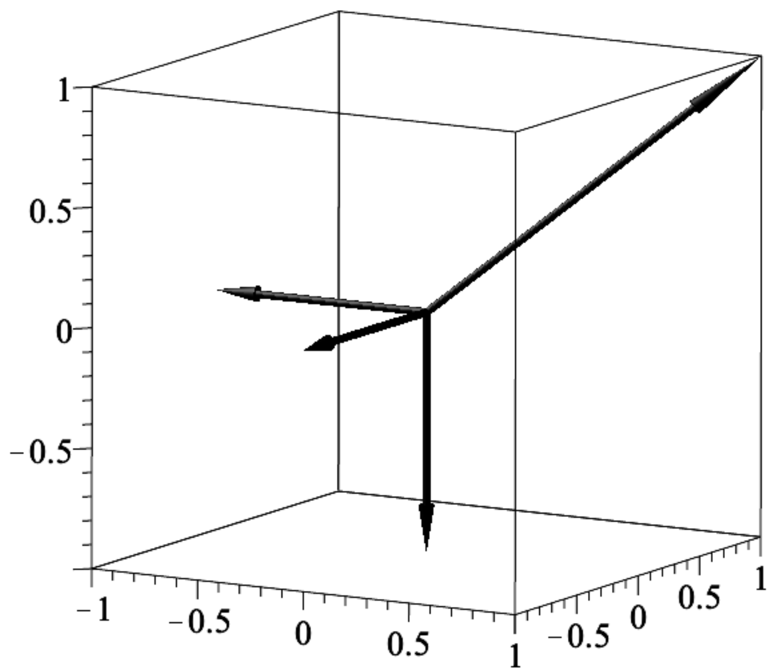
Contradiction.



[BostanRaschelSalvy14]

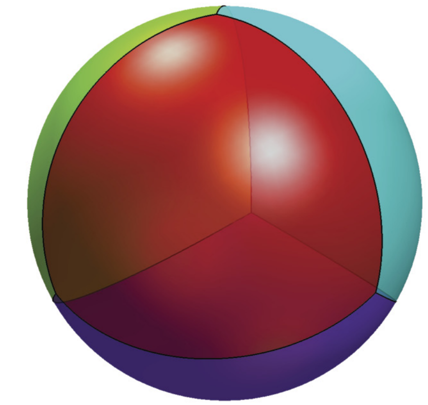
Example: Kreweras 3D

The group of the walk is finite



$$\mathcal{S} = \left\{ \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right\}$$

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



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$(2\pi/3, 2\pi/3, 2\pi/3)$

Previous estimates lead to:

$\alpha_\kappa \in [3.323, 3.326]$ (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)

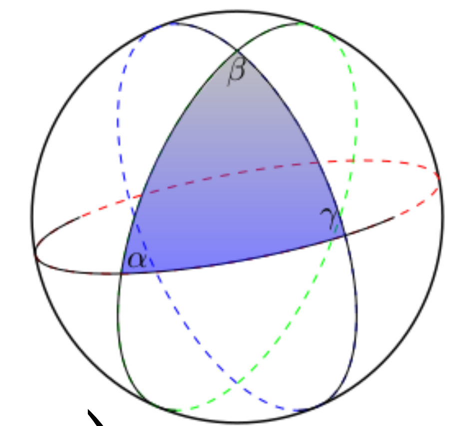
New: $\alpha_\kappa \simeq 3.3257570041744562 5097\ldots \pm 10^{-101}$

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

D-finiteness more and more doubtful

II. 3D Walks: Laplacian on Spherical Triangles

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:

. $(2,3,3) \longrightarrow \lambda = k(k+1),\ k \in 6 + 3\mathbb{N} + 4\mathbb{N}$

. $(2,3,4) \longrightarrow \lambda = k(k+1),\ k \in 9 + 6\mathbb{N}$

. $(2,3,5) \longrightarrow \lambda = k(k+1),\ k \in 15 + 6\mathbb{N} + 10\mathbb{N}$

. $(2,2,r) \longrightarrow \lambda = k(k+1),\ k \in r + 1 + 2\mathbb{N} + r\mathbb{N}$

This solves 7 of the 17 spherical triangles with finite groups

$$-\frac{p}{2} := \sqrt{\lambda_1 + (d/2-1)^2} + 1 \in \mathbb{Q}$$

No other value known —> turn to numerical computation

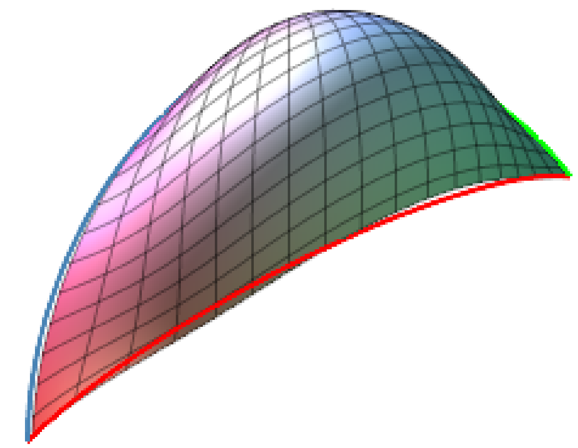
[Berard1983,BogoselPerrollazRaschelTrotignon20]

Bounds from an Approximate Eigenvalue

Eigenvalue problem for Ω :

$$\Delta f + \lambda f = 0 \text{ in } \Omega, \quad f|_{\partial\Omega} = 0.$$

replace by f small



Thm. If $\Delta f^\star + \lambda^\star f^\star = 0$ in Ω, then there exists λ s.t.

$$\frac{|\lambda - \lambda^\star|}{\lambda} \leq \frac{\sup_{x\in\partial\Omega} |f^\star(x)|}{\|f^\star\|_2}.$$

Method:

1. Find a good approximate pair $(f^\star, \lambda^\star)$
2. Upper bound $\sup_{x\in\partial\Omega} |f^\star|$ in a certified way
3. Lower bound $\|f^\star\|_2$ in a certified way
4. Certify the index

Only 1. & 2. in this talk (most of the time in the computation)

[FoxHenriciMoler67,MolerPayne68]

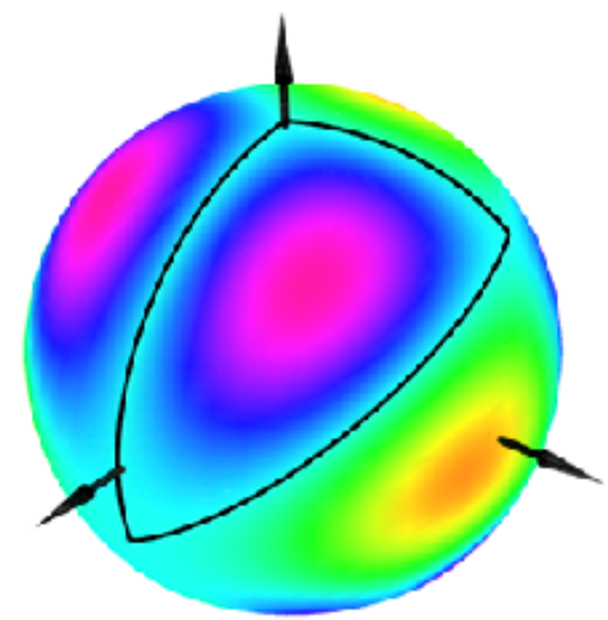
Step 1. Find a good approximate pair $(f^\star, \lambda^\star)$

$$\frac{|\lambda - \lambda^\star|}{\lambda} \leq \frac{\sup_{x\in\partial\Omega} |f^\star(x)|}{\|f^\star\|_2}.$$

High precision needed, and no guarantee

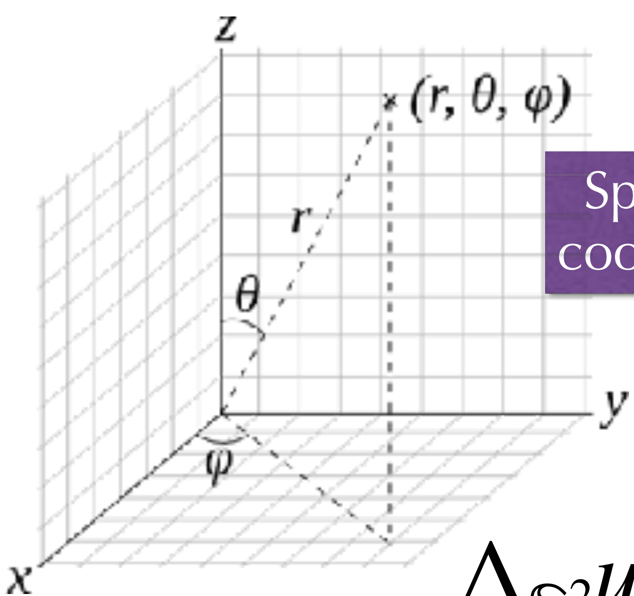
Method of Particular Solutions

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
   . small on $\partial\Omega$
   . *not too small on* Ω
4. Repeat to minimize $\sup_{x\in\partial\Omega}$ over λ

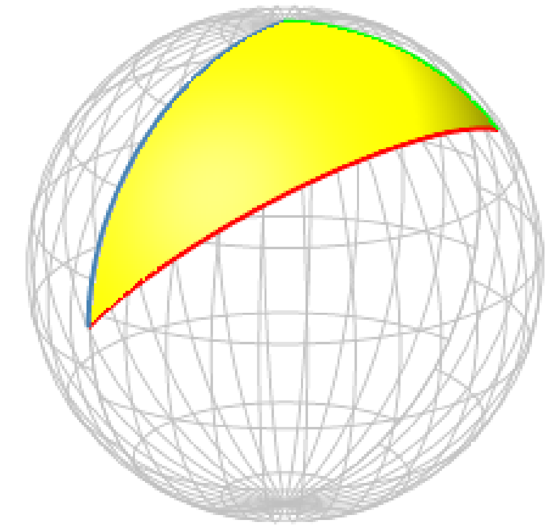


[Bergman47,Vekua48,FoxHenriciMoler67,BetckeTrefethen05,Betcke08]

2. Set of Eigenfunctions



Spherical coordinates



$$\Delta_{\mathbb{S}^2} u(\theta,\phi) = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}$$

Separation of variables gives

$$\boxed{u_\lambda^{(k)}(\theta,\phi) = \sin(\mu_k\phi)\,\mathsf{P}_\nu^{\mu_k}(\cos\theta)}$$

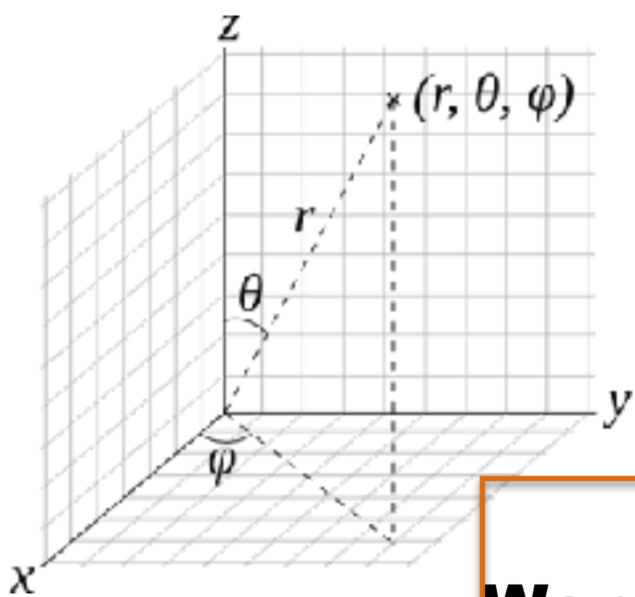
Ferrers function of the 1st kind (D-finite; generalize the Legendre functions)

with $\lambda = \nu(\nu+1)$, $\quad \mu_k := -\frac{k\pi}{\phi_{\max}},\ k \in \mathbb{N}$

$$u_\lambda^{(k)}(\theta,0) = u_\lambda^{(k)}(\theta,\phi_{\max}) = 0.$$

One edge of the triangle left

3. Last Part of the Boundary

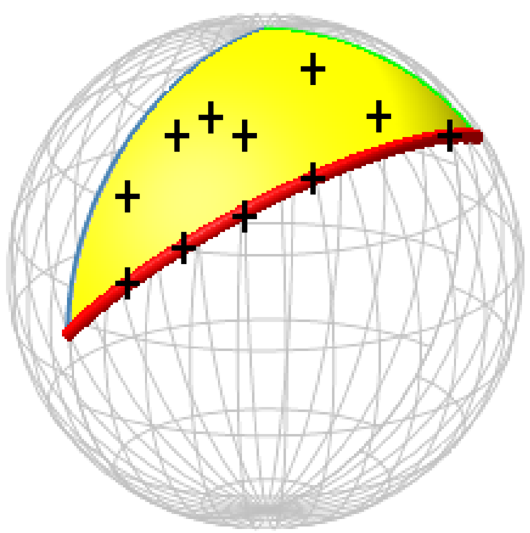


$$u_\lambda(\phi) := \sum_{k=1}^{N} c_k \sin(\mu_k \phi) \mathrm{P}_\nu^{\mu_k}(\cos\theta(\phi))$$

with $\lambda = \nu(\nu+1)$

satisfies $\Delta u_\lambda + \lambda u_\lambda = 0$

$\boxed{\textbf{Wanted: } c_k \text{ s.t. } u_\lambda|_{[0,\phi_{\max}]} \approx 0,\ \|u_\lambda\|_\Omega \approx 1.}$



Choose $x_1, \ldots, x_{m_b}$ on $\partial\Omega$, $y_1, \ldots, y_{m_i}$ inside Ω;

Form a matrix $A := \begin{pmatrix} u_\lambda^{(k)}(x_i) \\ u_\lambda^{(k)}(y_i) \end{pmatrix}$

Orthonormal basis of Im A

Compute its QR factorization $A = \begin{pmatrix} Q_{\partial\Omega} \\ Q_\Omega \end{pmatrix} R$

$\sigma := \min_{\|v\|=1} \|Q_{\partial\Omega} v\|$ found together with v by SVD (least squares)

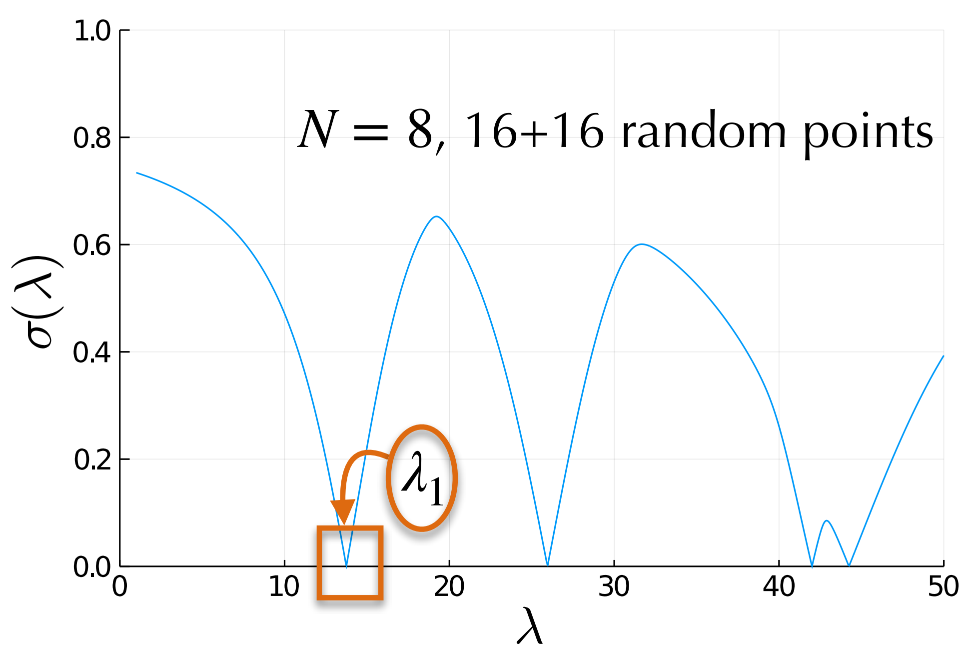
Then $\|Q_\Omega v\|^2 = 1 - \sigma^2$ not too small

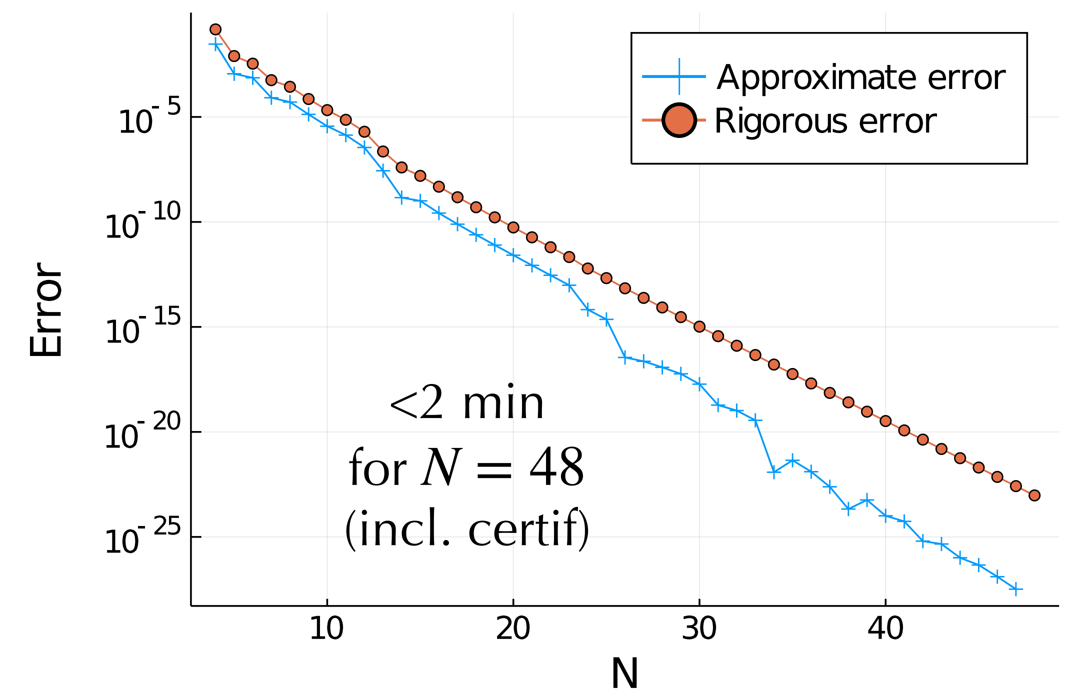
Recover c by solving $Rc = v$.

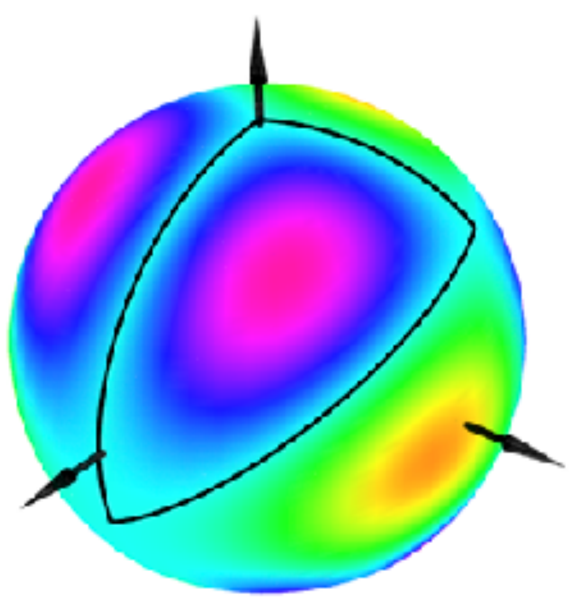
[BetckeTrefethen05]

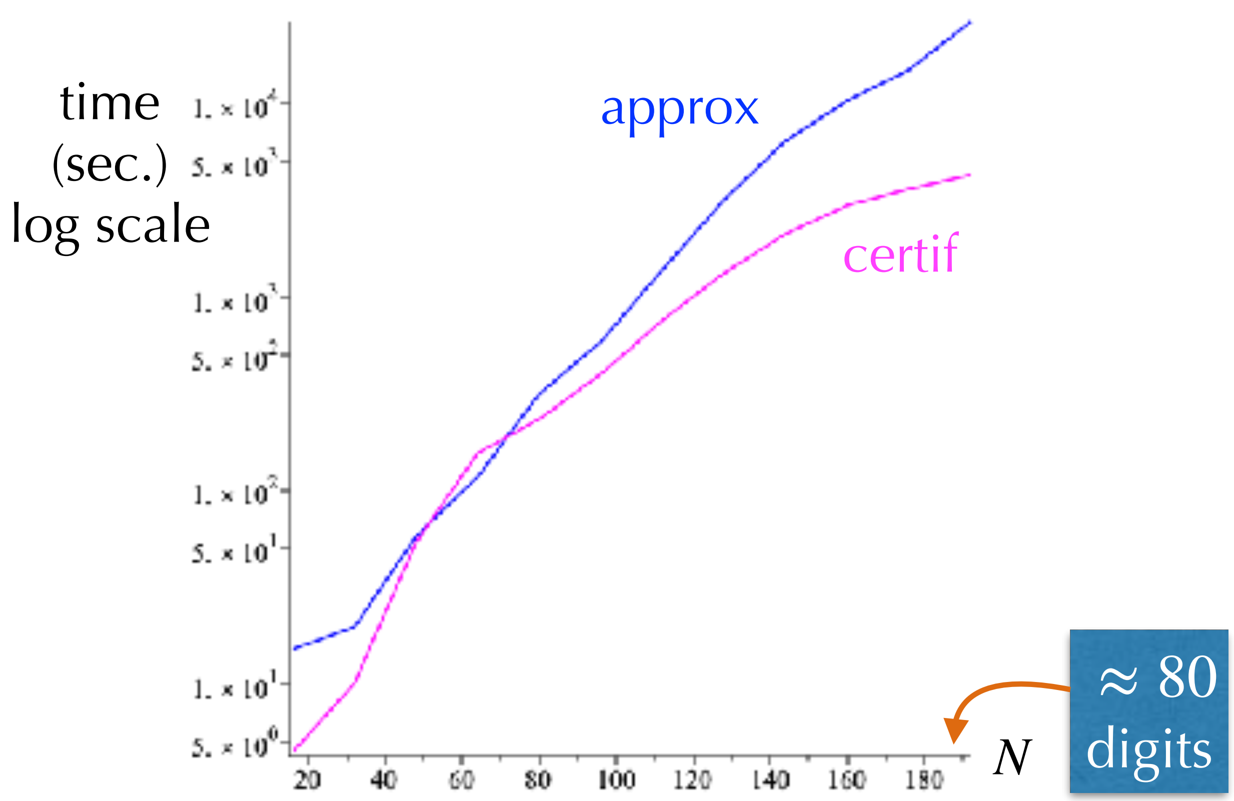
4. Optimize over λ

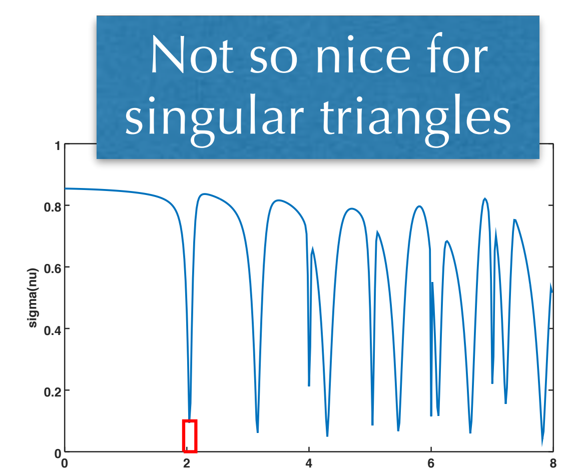
Ex. Regular Triangle: $(2\pi/3, \pi/3, \pi/2)$











$(\pi/2, 2\pi/3, 3\pi/4)$

1. Find a good approximate pair $(f^\star, \lambda^\star)$
2. Upper bound $\sup_{x\in\partial\Omega} |f^\star|$ in a certified way
3. Lower bound $\|f^\star\|_2$ in a certified way
4. Certify the index

Step 2. Upper 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 https://arblib.org/

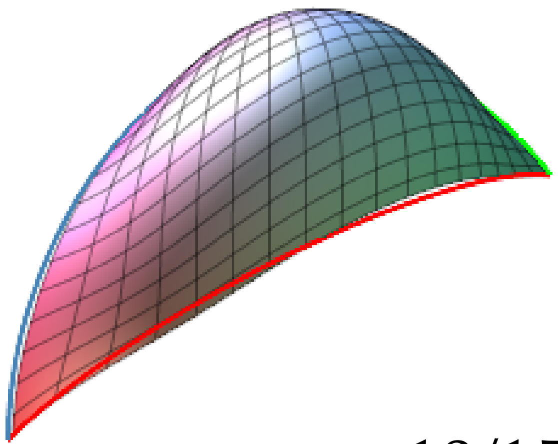
Weakness: wrapping effect

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

$f([1.0,1.1]) = [-0.161,0.161]$ 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 $\partial\Omega$



Upper Bound on the Boundary

$$\frac{|\lambda - \lambda^\star|}{\lambda} \leq \frac{\sup_{x\in\partial\Omega} |f^\star(x)|}{\|f^\star\|_2}$$

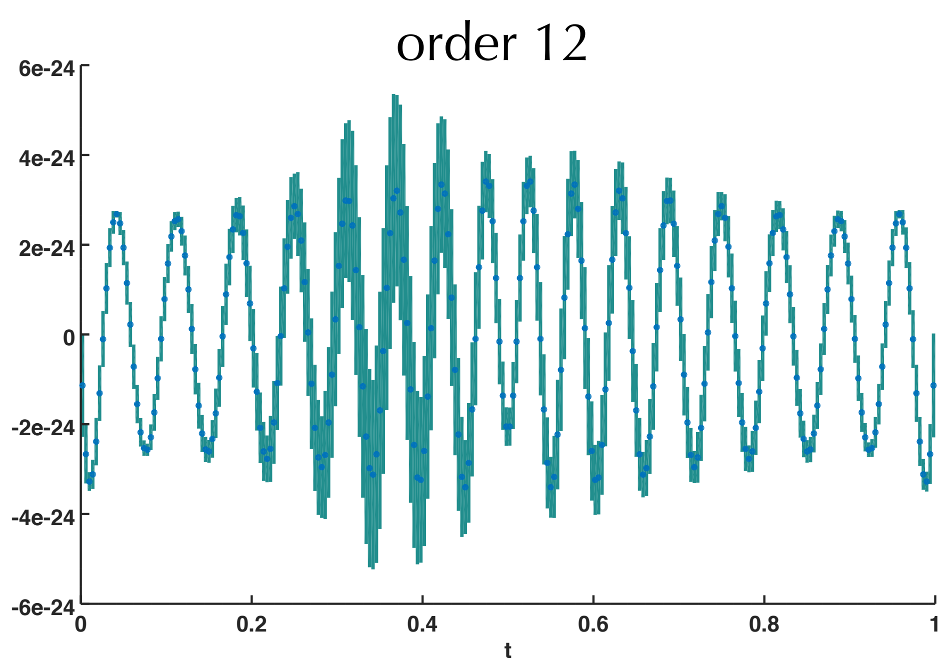
Taylor model:

$$\max_{t\in I} f^\star(\gamma(t)) \leq \max_{t\in I} P_{\ell-1}(t) + \boxed{\frac{(|I|/2)^\ell}{\ell\,!}} \max_{t\in I} \left| \frac{d^\ell}{dt^\ell} f^\star(\gamma(t)) \right|$$

Taylor expansion at the midpoint
Coefficients via linear rec.

small

interval evaluation



A lower bound on $\min f^\star$ also follows

Interval-evaluate
at enclosures of roots of the
derivative

The expensive part of the certification

[MakinoBerz03]

Results

Angles	BPRT	new	bound denom
$(3\pi/4,\pi/3,\pi/2)$	12.400051	$12.40005165284337790 5\ldots \pm 10^{-47}$	10^{23}
$(2\pi/3,\pi/3,\pi/2)$	13.744355	$13.7443552132132318 35\ldots \pm 10^{-84}$	10^{40}
$(2\pi/3,\pi/4,\pi/2)$	20.571973	$20.5719735379847305 57\ldots \pm 10^{-30}$	10^{14}
$(2\pi/3,\pi/3,\pi/3)$	21.309407	$21.3094076301904452 60\ldots \pm 10^{-206}$	10^{103}
$(3\pi/4,\pi/4,\pi/3)$	24.456913	$24.4569137962991116 94\ldots \pm 10^{-73}$	10^{37}
$(2\pi/3,\pi/4,\pi/4)$	49.109945	$49.1099452632846099 20\ldots \pm 10^{-153}$	10^{76}
$(2\pi/3,3\pi/4,3\pi/4)$	4.261734	$4.2617347552939870857\ldots \pm 10^{-22}$	10^{10}
$(2\pi/3,2\pi/3,2\pi/3)$	5.159145	$5.1591456424665417112\ldots \pm 10^{-104}$	10^{51}
$(\pi/2,2\pi/3,3\pi/4)$	6.241748	$6.2417483307263342368\ldots \pm 10^{-20}$	10^{9}
$(\pi/2,2\pi/3,2\pi/3)$	6.777108	$6.7771080545983009573\ldots \pm 10^{-35}$	10^{17}

finite elements &
convergence acceleration

more work
for this one

[BogoselPerrollazRaschelTrotignon20,DahneSalvy20]

Summary & Conclusion

Numerical computation can yield rigorous results, useful in experimental mathematics.

See the article for more on:

lower bounding the norm;
certifying the index;
singular vs regular triangles.

Thank you.