Spherical cap discrepancy of perturbed lattices under the Lambert projection

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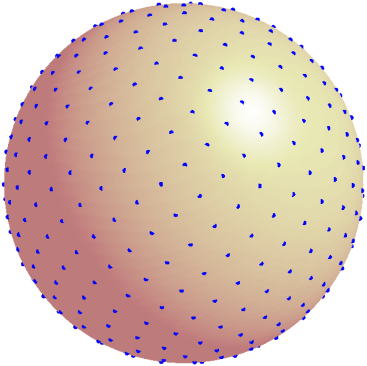
Setting the Stage

History

In 1904, physicist and Nobel Prize winner J. Thomson worked on a model of the atom – this led to the question: which configuration of electrons on a spherical shell would minimize electrostatic potential energy. Known configurations for $N \in \{1, 2, 3, 4, 5, 6, 12\}$.

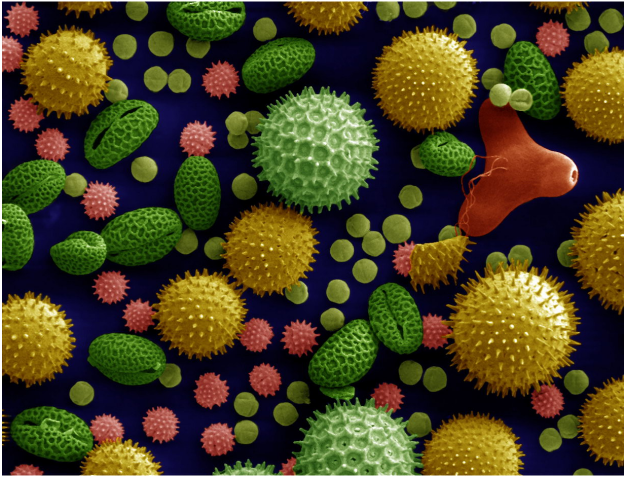


Coulomb Potential: Given a point set $\omega_N := \{x_1, \dots, x_N\}$ on the sphere, minimize

$$\sum_{j \neq k} \frac{1}{\|x_j - x_k\|}.$$

History

In 1930, botanist P. Tammes observed equally spread out pores on pollen grains – this led to the question of maximizing the smallest distance between any two pores.



Public Domain picture of pollen grains from Wikipedia. (Dartmouth Electron Microscope Facility, Dartmouth College.)

Applications

Material Science

Two-Dimensional Matter: Order, Curvature and Defects – M. Bowick and L. Giomi, Advances in Physics (58) (2009).

Physics

Ground State Energy of Unitary Fermion Gas with the Thomson Problem Approach – Chen Ji-Sheng, Chinese Phys. Lett. 24 1825 (2007).

Virology

Why large icosahedral viruses need scaffolding proteins – S. Li, P. Roy, A. Travesset and R. Zandi, PNAS, (43) 115 (2018).

Pattern Formation in Icosahedral Virus Capsids: The Papova Viruses and Nudaurelia Capensis β Virus – C. Marzec and L. Day, Biophysical Journal (65) (1993).

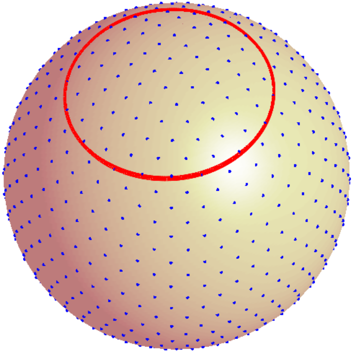
Equidistribution

Spherical Cap with center $w \in \mathbb{S}^2$ and height $t \in [-1, 1]$ is

$$C(w, t) = \{x \in \mathbb{S}^2 \; : \; \langle x, w \rangle \geq t\}.$$

Normalized uniform measure is σ.

Let $\omega_N = \{z_1, \ldots, z_N\} \subset \mathbb{S}^2$, define

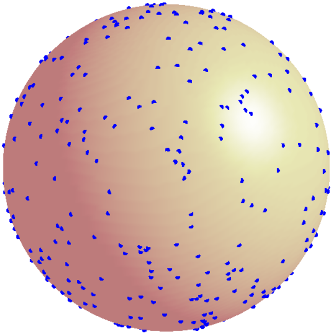


$$\mathcal{D}(\omega_N) = \sup_{w \in \mathbb{S}^2} \sup_{-1 \leq t \leq 1} \left| \frac{1}{N} \sum_{j=1}^{N} \chi_{C(w,t)}(z_j) - \sigma(C(w, t)) \right|.$$

Integration Error

Let f be a function of bounded Variation* and ω_N as earlier, then the Koksma – Hlawka inequality is

$$\left| \frac{1}{N} \sum_{j=1}^{N} f(z_j) - \int f \,\mathrm{d}x \right| \leq \mathcal{D}(\omega_N)\mathcal{V}(f).$$



For i.i.d. random points wrt. σ

$$\mathcal{D}(\omega_N) \sim \frac{1}{\sqrt{N}}.$$

A general theorem from the theory of uniform distribution modulo 1 – F. Koksma, Mathematica B (Zutphen), 11 (1942).

Equidistribution and energy minimization I

Theorem (Marzo+Mas 2021)

Let $\omega_N^\star \subset \mathbb{S}^d$ denote a minimizer of the Riesz s-energy, $0 < s < d$, then

$$\mathcal{D}(\omega_N^\star) \;\leq\; 1_{(0,d-2]}(s) C_{s,d} N^{-\frac{2}{d(d-s+1)}} + 1_{(d-2,d)}(s) C_{s,d} N^{-\frac{2(d-s)}{d(d-s+4)}}.$$

$\star$ Marzo, Mas: *Discrepancy of Minimal Riesz Energy Points*. Constructive Approximation 54, pp. 473–506 (2021).

Equidistribution and energy minimization II

Theorem (Brauchart 2008)

Let $\omega_N^\star \subset \mathbb{S}^d$ denote a minimizer of the Logarithmic Energy, then

$$\mathcal{D}(\omega_N^\star) \;=\; O\big(N^{\frac{-1}{d+2}}\big).$$

$\star$ Brauchart: *Optimal Logarithmic Energy Points*. Mathematics of Computation Vol. 77 (263), (2008).

Known constructions with low cap discrepancy

Spherical digital nets and Fibonacci lattices

⋆ Aistleitner, Brauchart, Dick: *Point Sets on the Sphere S_2 with Small Spherical Cap Discrepancy*. Discrete Comput Geom 48, pp. 990-1024 (2012).

Diamond ensamble

⋆ Etayo: *Spherical Cap Discrepancy of the Diamond Ensemble*. Discrete Comput Geom (2021).

HEALPix

⋆ DF, Hofstadler, Mastrianni: *The spherical cap discrepancy of HEALPix points*. arXiv (2022).

Beck's result

Theorem (Beck 1984)

$$cN^{-3/4} \leq \mathcal{D}(\omega_N^\star) \leq CN^{-3/4}\sqrt{\log N}.$$

Task: Prove an upper bound on the spherical cap discrepancy for a deterministic algorithm of order less than $N^{-1/2}$.

Question: Does "good" spherical cap discrepancy implies "good" Riesz/Logarithmic energy?

Result and Proof Idea

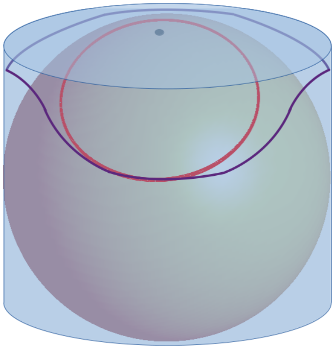
The Lambert projection

We define $L : (0,1)^2 \to \mathbb{S}_p^2$

$$(x,y) \mapsto \begin{pmatrix} 2\sqrt{y-y^2}\cos(2\pi x) \\ 2\sqrt{y-y^2}\sin(2\pi x) \\ 1-2y \end{pmatrix},$$

and L^{-1} via

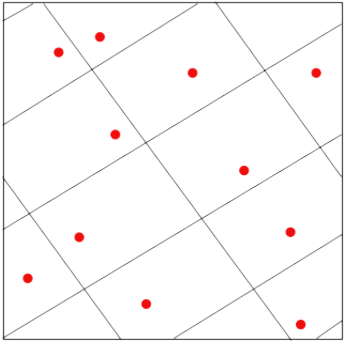
$$\begin{pmatrix} \cos(\phi)\sin(\theta) \\ \sin(\phi)\sin(\theta) \\ \cos(\theta) \end{pmatrix} \mapsto \begin{pmatrix} \frac{1}{2\pi}\phi \\ \frac{1-\cos(\theta)}{2} \end{pmatrix}.$$



L is area preserving! We set for $Q \in \mathrm{GL}(\mathbb{R}^2)$

$$C_L^Q = \sup_{w \in S_2} \sup_{-1 \le t \le 1} \mathrm{length}\Big(Q^{-1}\big(L^{-1}(\partial C(w,t))\big)\Big).$$

Defining points $P^Q(K)$



A lattice is $Q\mathbb{Z}^2$ for $Q \in \mathrm{GL}(\mathbb{R}^2)$,

$$\mathbb{R}^2 = \bigcup_{p \in Q\mathbb{Z}^2} \frac{1}{K}\left(p + Q[0,1)^2\right).$$

$$z_K^p \in \frac{1}{K}(p + Q[0,1)^2)$$

for $K \in \mathbb{N}$, and $p \in Q\mathbb{Z}^2$, and set

$$P^Q(K) = \left\{z_K^p \mid p \in Q\mathbb{Z}^2\right\} \cap [0,1)^2.$$

Let $N^Q(K) = \#P^Q(K)$ and set

$$d^Q(K) = \frac{1}{K}\left|N^Q(K) - \frac{K^2}{|\det(Q)|}\right|.$$

Main result

Theorem (DF 2022)

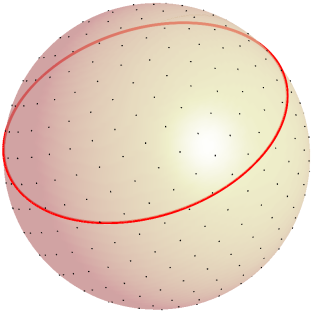
Let $Q \in \mathrm{GL}(\mathbb{R}^2)$, $K \in \mathbb{N}$ and $N = N^Q(K)$, then

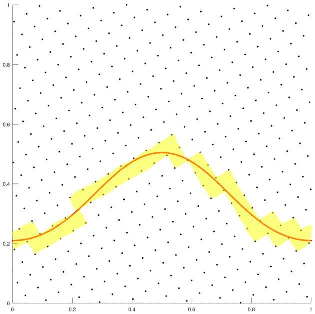
$$\mathcal{D}(L(P^Q(K))) \ \leq \ \left(d^Q(K) + \sqrt{2} \cdot C_L^Q\right) \frac{\sqrt{|\det(Q)|}}{\sqrt{N}} + O(N^{-1}).$$

Blueprint for a Proof I

$$\left|\frac{1}{N}\sum_{j=1}^{N}1_{C(w,t)}(z_j)-\sigma(C(w,t))\right| = \left|\frac{1}{N}\sum_{j=1}^{N}\chi_{L^{-1}(C(w,t))}(z_j)-\sigma(C(w,t))\right|$$

$$\leq \left|\frac{1}{N}\sum_{p_j\in V}\chi_{L^{-1}(C(w,t))}(z_j)-\sum_{p_j\in V}\lambda\big(T_K(p_j)\big)\right|+\sum_{q\in B}\lambda\big(T_K(q)\big).$$





Blueprint for a Proof II

The value

$$\Big|\frac{1}{N}\sum_{p_j\in V}\chi_{L^{-1}(C(w,t))}(z_j)-\sum_{p_j\in V}\lambda\big(T_K(p_j)\big)\Big|$$

can be bounded by the sum of small errors, of the form

$$|\epsilon_K| = \Big|\frac{1}{N}-\lambda(T_K(p_j))\Big| = \Big|\frac{1}{N}-\frac{|\det(Q)|}{K^2}\Big| \leq \frac{d^Q(K)|\det(Q)|}{KN}.$$

There are at most N such error terms, resulting in the bound

$$\frac{d^Q(K)|\det(Q)|}{K}.$$

An estimate on the number of intersections of fundamental domains with $L\circ\partial C$ bounds

$$\sum_{q\in B}\lambda\big(T_K(q)\big).$$

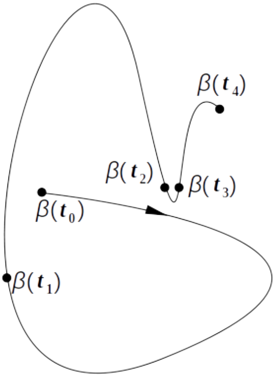
The Intersection Lemma

n convex curves

We call a continuous curve $\beta : [a, b] \to \mathbb{R}^2$ n-convex for $n \in \mathbb{N}$, if

$$a = t_0 < t_1 < \ldots < t_{n-1} < t_n = b$$

and $\beta\big([t_j, t_{j+1}]\big)$ is convex.



The backbone of the paper

Lemma (DF '22) Let β be a piece-wise $\mathcal{C}^1$-curve in $\mathbb{R}^2$ and *n*-convex, then the intersection number $I_\beta^Q(K)$ of β with $\frac{1}{K}Q\mathbb{Z}^2$ ($K \in \mathbb{N}$) satisfies

$$I_\beta^Q(K) \ \leq \sqrt{2} \cdot \mathrm{length}\big(Q^{-1}\beta\big) \cdot K + 19n + 1.$$

Proof of the lemma: monotonicity I

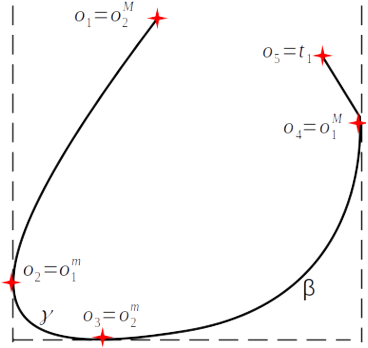
Let $Q = \mathrm{id}$ and β be $\mathcal{C}^1$.

Choose $M_j, m_j \in \beta\big([0, t_1]\big)$ such that

$$\langle M_j, e_j\rangle = \max_{t\in[0,t_1]} \langle \beta(t), e_j\rangle$$

and

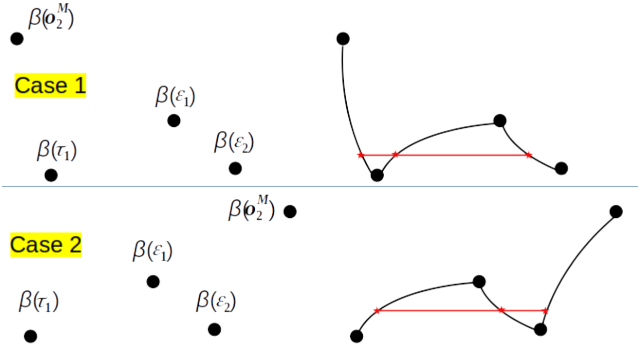
$$\langle m_j, e_j\rangle = \min_{t\in[0,t_1]} \langle \beta(t), e_j\rangle.$$



Choose $o_j^M \in \beta^{-1}(M_j) \cap [0, t_1]$ and $o_j^m \in \beta^{-1}(m_j) \cap [0, t_1]$ for $j \in \{1, 2\}$. Let o_1, o_2, o_3, o_4 denote these o_j^m, o_j^M in ascending order.

Proof of the lemma: monotonicity II

Let $[\tau_1, \tau_2]$ be a pair $[o_j, o_{j+1}]$, and wlog. $\beta(\tau_1) = m_2$.
The existence of numbers $\tau_1 < \epsilon_1 < \epsilon_2 < \tau_2$ such that $y(\epsilon_1) > y(\epsilon_2)$ will lead to a contradiction.



Proof of the lemma: monotonicity III

Let $[\tau_1, \tau_2]$ be a pair $[o_j, o_{j+1}]$, and wlog. $\beta(\tau_1) = m_2$.
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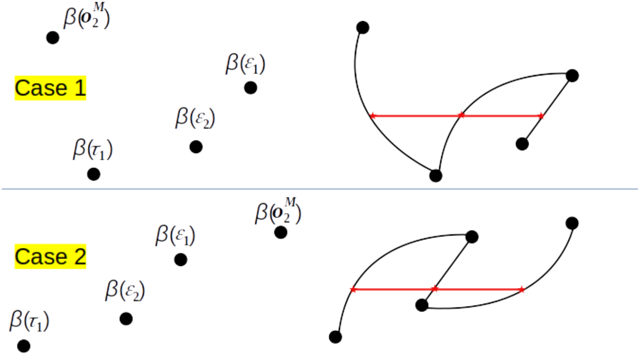


Proof of the lemma: intersection count

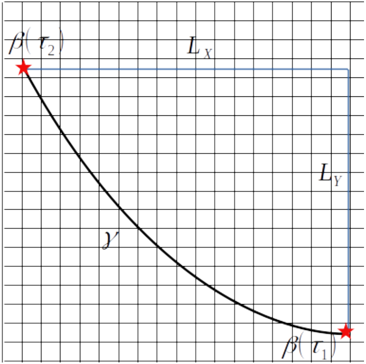
By monotonicity

$$I_\gamma^{\mathrm{id}}(K) \ \leq \ I_{L_x}^{\mathrm{id}}(K)+I_{L_y}^{\mathrm{id}}(K) \ \leq \ (c+d)K+4$$

with $\mathrm{length}(L_x) = c$ and $\mathrm{length}(L_y) = d$. We further use

$$c + d \leq \sqrt{2}\sqrt{c^2 + d^2}$$

to derive



$$I_\gamma^{\mathrm{id}}(K) \ \leq \ \sqrt{2}\sqrt{c^2 + d^2} \cdot K + 4 \ \leq \ \sqrt{2}\,\mathrm{length}(\gamma) \cdot K + 4.$$

Generalize to Q.□

Concrete Bounds

Estimates on C_L^Q

L the Lambert map. We set for $Q \in \mathrm{GL}(\mathbb{R}^2)$

$$C_L^Q = \sup_{w \in S_2} \sup_{-1 \le t \le 1} \mathrm{length}\Big(Q^{-1}\big(L^{-1}\big(\partial C(w,t)\big)\big)\Big).$$

Lemma Given a matrix A and a $\mathcal{C}^1$-curve β in $\mathbb{R}^2$, then with
$\ell_\beta = \mathrm{length}(\beta)$,
$\ell_A = \mathrm{length}(A\beta)$,
$m_A = \min\{\|Ae_1\|, \|Ae_2\|\}$ and
$M_A = \max\{\|Ae_1\|, \|Ae_2\|\}$ we have

$$\begin{aligned} m_A \cdot \ell_\beta \le \ell_A &\le M_A \cdot \ell_\beta && \text{if } A \text{ has rank 2 and } A \text{ orthogonal,} \\ \ell_A &\le \|A\|_F \cdot \ell_\beta && \text{if } A \text{ has rank 2.} \end{aligned}$$

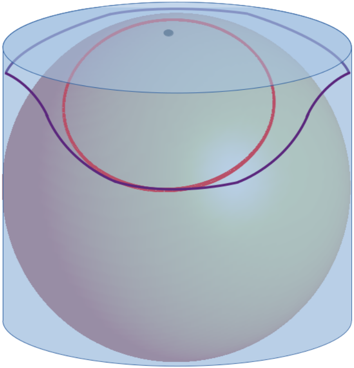
Bounding C_L^{id} I

Lemma $C_L^{\mathrm{id}} \leq 3$.

We let z_1, z_2 approach ± 1 and regard $C(w, 0)$ with

$$w = \left(\sin\left(\frac{\pi}{2} - \epsilon\right), 0, \cos\left(\frac{\pi}{2} - \epsilon\right)\right)^t$$

and $\epsilon > 0$ small.



Bounding C_L^{id} II

A parametrization for $\partial C(w,0)$ is then given by

$$\begin{aligned}\varphi_\pm : [\epsilon, \pi-\epsilon] &\to [0, 2\pi]\\ \theta &\mapsto \pm\arccos\big(-\cot(\theta)\cot\big(\tfrac{\pi}{2}-\epsilon\big)\big);\end{aligned}$$

such that

$$\begin{aligned}\gamma_+ : [\epsilon, \pi-\epsilon] &\to \partial C(w,0)\\ \theta &\mapsto \begin{pmatrix}\cos\big(\varphi_+(\theta)\big)\sin(\theta)\\ \sin\big(\varphi_+(\theta)\big)\sin(\theta)\\ \cos(\theta)\end{pmatrix}.\end{aligned}$$

$L^{-1}\circ\gamma_+$ and $L^{-1}\circ\gamma_-$ have the same length, thus we regard the curve

$$\frac{1}{\pi}\begin{pmatrix}\arccos\big(-\cot(\theta)\cot\big(\tfrac{\pi}{2}-\epsilon\big)\big)\\ \pi(1-\cos(\theta))\end{pmatrix}.$$

Bounding C_L^{id} III

$$\mathrm{length} = \int_{\epsilon}^{\pi-\epsilon} \sqrt{\frac{1}{1-\cot(\theta)^2 \cot\left(\frac{\pi}{2}-\epsilon\right)^2} \frac{\cot\left(\frac{\pi}{2}-\epsilon\right)^2}{\pi^2 \sin(\theta)^4} + \sin(\theta)^2}\ \mathrm{d}\theta.$$

Simplify the expression with the angle sum formula for the cosine (with $\epsilon < \theta < \pi - \epsilon$) and with $\cos\left(\epsilon - \frac{\pi}{2}\right) = \sin(\epsilon)$ and a symmetry argument to get

$$\mathrm{length} = 2 \int_{\epsilon}^{\frac{\pi}{2}} \sqrt{\frac{1}{\sin(\epsilon+\theta)\sin(\theta-\epsilon)} \frac{\sin(\epsilon)^2}{\pi^2 \sin(\theta)^2} + \sin(\theta)^2}\ \mathrm{d}\theta.$$

Bounding C_L^{id} IV

$$\mathrm{length} = 2\int_{\epsilon}^{\frac{\pi}{2}} \sqrt{\frac{1}{\sin(\epsilon+\theta)\sin(\theta-\epsilon)}\frac{\sin(\epsilon)^2}{\pi^2\sin(\theta)^2} + \sin(\theta)^2}\ \mathrm{d}\theta.$$

For any choice of $a \in (0, \frac{\pi}{2}]$, we have

$$\mathrm{sinc}(a)\ x \leq \sin(x) \leq x,\ \text{ for } x \in [0, a];$$

$$\mathrm{length} \leq \frac{2}{\mathrm{sinc}(a)^2\pi}\int_{\epsilon}^{a-\epsilon} \sqrt{\frac{1}{\theta^2-\epsilon^2}\frac{\epsilon^2}{\theta^2}}\ \mathrm{d}\theta + \frac{\epsilon\cdot\pi^2}{4\sqrt{a(a-2\epsilon)^3}} + 2\int_{\epsilon}^{\frac{\pi}{2}} \sin(\theta) d\theta$$

$$= \frac{2}{\mathrm{sinc}(a)^2\pi}\int_{1}^{a/\epsilon-1} \sqrt{\frac{1}{x^2-1}}\frac{1}{x}\ \mathrm{d}x + O(\epsilon) + 2 \overset{\lim \epsilon\to 0}{\leq} \frac{2}{\mathrm{sinc}(a)^2\pi}\frac{\pi}{2} + 2. \square$$

An Example

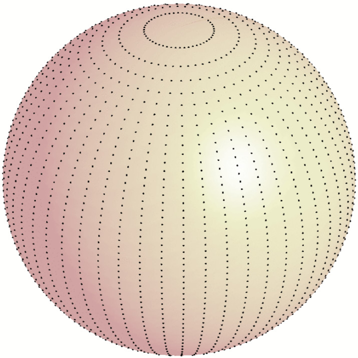
Best leading constant

$P(K) = \left(\frac{1}{K}\mathbb{Z}^2 + \frac{1}{2K}\binom{1}{1}\right) \cap [0,1]^2.$

Then $N = K^2$, and thus $d(K) = 0$,

$$\frac{1}{4} \;\le\; \sqrt{N} \cdot \mathcal{D}(L(P^1(K))) \;\le\; \sqrt{18}.$$

The lower bound comes from a special choice for a spherical cap: take as center the north pole and let the height $t \to \frac{2K-1}{2K}^{+}$.



Thank you for your Time