

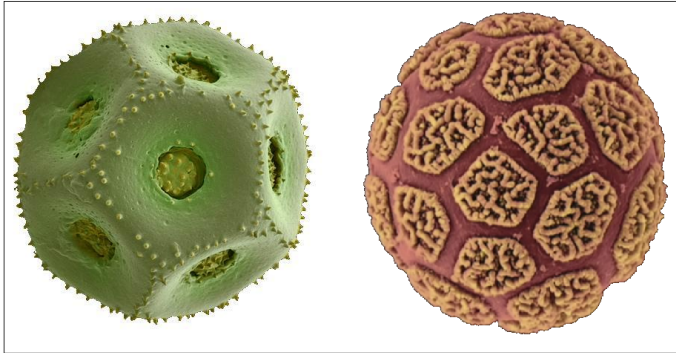
Heating the sphere

Carlos Beltrán

Universidad de Cantabria, Santander

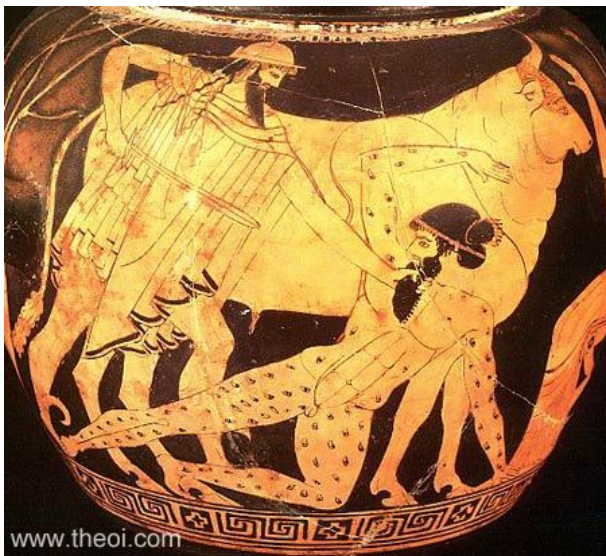
Foundations of Computational Mathematics 2014, Montevideo

Gimme points



Pollen particles: *stellaria holostea* and *iris decora*. Rob Kessler and Madeline Harley

Little history and incomplete list of researchers involved.



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- Thomson's problem. J. J. Thomson, 1904. **Energy minimization** and more: see references in next slices.
- Tammes problem (1930). Habicht, Schutte, van der Waerden, Danzer, Fejes Toth, Cohn, Jiao, Kumar, Torquato, Brauchart, Dick, Saff, Sloan, Wang, Womersley,
- Quadrature formulas (spherical N -designs), spherical harmonics and interpolation. Hesse, Sloan, Womersley, Aistleitner, Brauchart, Dick, Bondarenko, Radchenko, Viazovska
- Maximal distance sums. Alexander, Beck, Stolarski.
- Number Theory and Arakelov Theory. Elkies, Baker.
- One component plasma Coulomb gases at zero temperature. Sandiers, Serfaty.
- ESI Programme <http://www.math.tugraz.at/ESI2014/>

Points satisfying some “extremal” property

A frequent choice

Look for N points x_1, \dots, x_N in the sphere \mathbb{S} such that the logarithmic energy (aka logarithmic potential)

$$\mathcal{E}(x_1, \dots, x_N) = \log \prod_{i < j} \|x_i - x_j\|^{-1} = - \sum_{i < j} \log \|x_i - x_j\|$$

is minimized.

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is minimized.

A set of N points in \mathbb{S} minimizing \mathcal{E} (i.e. maximizing the product of their mutual distances) is called a set of **Elliptic Fekete Points**.

Elliptic Fekete points

Early works by Fekete, Szegő, Whyte, Hille, Tsuji, etc.

For $X = (x_1, \dots, x_N) \in \mathbb{S}^N$ where $x_i \in \mathbb{S}$, $1 \leq i \leq N$, elliptic Fekete points minimize the logarithmic energy

$$\mathcal{E}(X) = \mathcal{E}(x_1, \dots, x_N) = \log \prod_{i < j} \|x_i - x_j\|^{-1} = - \sum_{i < j} \log \|x_i - x_j\|$$

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Let

$$m_N = \min\{\mathcal{E}(X) : X \in \mathbb{S}^N\}.$$

Smale's 7th problem: can one find $X \in \mathbb{S}^N$ such that

$$\mathcal{E}(X) - m_N \leq c \log N?$$

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"Can one find" means...

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“Can one find” means...can one describe a polynomial time algorithm (BSS model)?

The minimal value of the energy.

Theorem (Elkies, Wagner, Rakhmanov–Saff–Zhou, Dubickas, Brauchart, Sandiers–Serfaty, Bétermin)

For the radius $1/2$ sphere, we have:

$$m_N = \frac{N^2}{4} - \frac{N \ln(N)}{4} + C_N N + o(N),$$

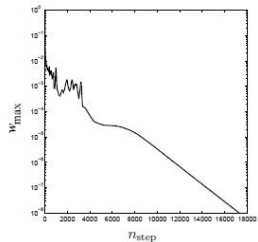
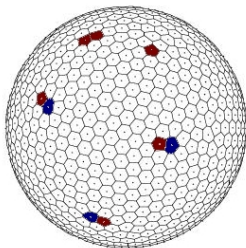
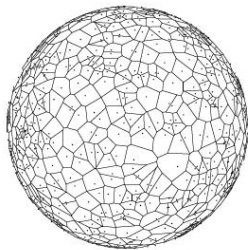
where

$$-0.4593423... \leq \lim_{N \rightarrow \infty} C_N \leq -0.40217...$$

Conjecture [Brauchart, Hardin, Saff; Serfaty et al]:

$$\lim_{N \rightarrow \infty} C_N = 2 \log 2 + \frac{1}{2} \log \frac{1}{3} + 3 \log \frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.40217...$$

Approximation to 1000 elliptic Fekete points by Bendito, Carmona, Encinas, Gesto, Gómez, Mouriño, Sánchez



We do know some things

Separation distance for the sphere of radius 1/2

- Theorem (Toth, Habicht– van der Waerden)

For the Tammes problem (maximize separation distance)

$$d_{\text{sep}}(X_{\text{Tammes}}) \approx \frac{1.9046\dots}{\sqrt{N}}.$$

- Theorem (Rakhmanov–Saff–Zhou, Dubickas, Dragnev)

For the elliptic Fekete points,

$$\frac{1}{\sqrt{N-1}} \leq d_{\text{sep}}(X_{\text{Fekete}}) \leq \frac{1.9046\dots}{\sqrt{N}}.$$

We do know some things

Baricenter [Bergersen-Boal-Palfy Muhoray], [Dragnev-Legg-Townsend]. True for any critical point of \mathcal{E} . [Brauchart] for the discrepancy, [Leopardi] for the comparison to s -energy.

Let x_1, \dots, x_N be a set of elliptic Fekete points.

- The baricenter of x_1, \dots, x_N is the center of the sphere.
- For each i ,

$$\sum_{j \neq i} \frac{x_i - x_j}{\|x_i - x_j\|^2} = 2(N-1)x_i, \quad \sum_{j \neq i} \|x_i - x_j\|^2 = \frac{N}{2}.$$

- Spherical cap discrepancy $cN^{-1/4}$ (see later).
- Asymptotically optimal s -energy in relative error (see later).

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Facility location problems

A modern classical subject on Optimization

Thanks to Giuseppe Buttazzo for a comment in the ADORT'10 meeting (Barcelona)

Facility location problems

A modern classical subject on Optimization

Choose N points in the 2 dimensional sphere \mathbb{S} in such a way that the average temperature in \mathbb{S} is the greatest possible.

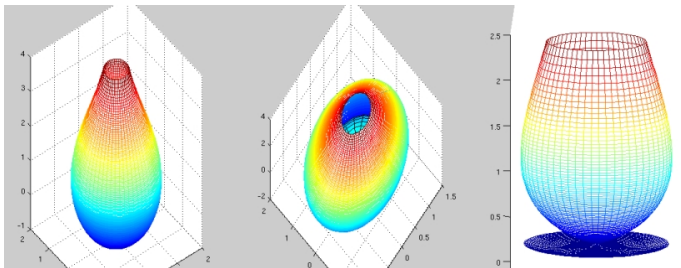
Here, the temperature $u = u(x, t)$ is assumed to satisfy the standard diffusion equation $u_t = \Delta u - \lambda$, where λ is a cooling rate, constant in \mathbb{S} , and the heat sources are assumed to be “infinite”.

The logarithm function in the sphere

The graphic corresponds to the function $x \mapsto -\log \|x - (0, 0, 1)\|$

Recall that \mathbb{S} is the Riemann sphere, that is the sphere of radius $1/2$ centered at $(0, 0, 1/2)$. Let

$$F_q : \mathbb{S} \setminus \{q\} \rightarrow \mathbb{R}$$
$$p \mapsto \log \|p - q\|^{-1}$$



The logarithm function in the sphere

Harmonic properties of the logarithmic energy

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$$F_q : \mathbb{S} \setminus \{q\} \rightarrow \mathbb{R}$$
$$p \mapsto \log \|p - q\|^{-1}$$

The (Riemannian) Laplacian of this function is constant:

$$\Delta F_q(p) = 2 \quad \forall p \in \mathbb{S} \setminus \{q\}.$$

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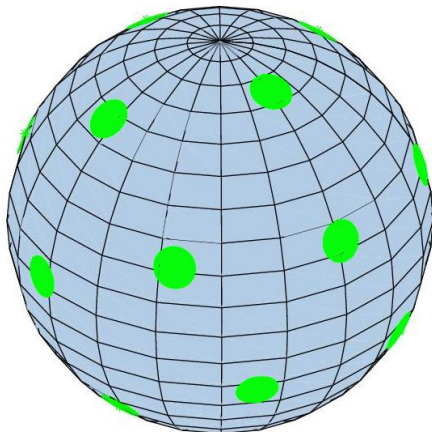
Here, the temperature $u = u(x, t)$ is assumed to satisfy the standard diffusion equation $u_t = \Delta u - \lambda$, where λ is a cooling rate, constant in \mathbb{S} , and the heat sources are assumed to be “infinite”.

After some assumptions on the rate of growth near the sources, the following stationary solution is found:

$$u(x) = u(x, t) = \frac{\lambda}{2N} \sum_{i=1}^N \log \|x_i - x\|^{-1} + u_0.$$

A new integral formula for the logarithmic energy [B. 2014]

Let $X = (x_1, \dots, x_N)$ be the center of the balls. Then, $\mathcal{E}(X)$ is up to a constant the integral in the grey part of a certain function.



A new integral formula for the logarithmic energy [B. 2014]

Let $X = (x_1, \dots, x_N) \in \mathbb{S}^N$.

Assume that caps of radius $\arcsin \sqrt{\delta/N}$ do not overlap.

Let

$B_0 =$ the grey area

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Then

$$\mathcal{E}(X) = \text{Constant}(N, \delta) - \frac{1-\delta}{2\delta} N \int_{x \in B_0} \sum_{i=1}^N \log \|x - x_i\|^{-1} dx. \quad (1)$$

An immediate consequence

Elliptic Fekete Points vs. Heat sources

Corollary

The following problems are equivalent:

- *The N -tuple $X = (x_1, \dots, x_N)$ is a set of elliptic Fekete points.*
- *For any $\delta \in (0, 1)$ and $r = \arcsin \sqrt{\delta/N}$ such that $d_R(x_i, x_j) \geq 2r$ for $i \neq j$, heat sources located at the points x_1, \dots, x_N maximize the average temperature out of a safety radius r around the sources.*

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Moreover... the total average temperature in \mathbb{S} is independent of the location of the sources.

Spherical cap discrepancy

Definition and theorems by Beck, Aistleitner, Brauchart, Dick, Gotz

$$D_C(X) = \sup_{x \in \mathbb{S}, r \in [0, \pi/2]} \left| \frac{\#\{i: x_i \in B(x, r)\}}{N} - \frac{\text{Area}(B(x, r))}{\pi} \right|.$$

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$$cN^{-3/4} \leq \min_X D_C(X) \leq CN^{-3/4} \log N.$$

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$$cN^{-3/4} \leq \min_X D_C(X) \leq CN^{-3/4} \log N.$$

If X is a set of Elliptic Fekete points,

$$D_C(X) \leq O(N^{-1/4}).$$

Spherical cap discrepancy

This follows from our main theorem

Theorem

Let $X \in \mathbb{S}^N$, $N \geq 2$ and let $\delta \in (0, 1)$ be such that $d_R(x_i, x_j) \geq 2 \arcsin \sqrt{\delta/N}$ for $i \neq j$. Then,

$$\mathcal{E}(X) \leq m_N + \frac{N^2}{4} D_C(X) \log \frac{N}{2\delta} + \frac{N \log(8\pi\delta)}{4}.$$

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Wagner proved a similar result for the case that we have the unit circle instead of \mathbb{S} .

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This is somehow a reciprocal of the known result that Elliptic Fekete points have small discrepancy [Brauchart] and are well-separated [Rakhmanov–Saff–Zhou, Dubickas, Dragnev].

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Theorem

Let $X \in \mathbb{S}^N$, $N \geq 2$ and let $\delta \in (0, 1)$ be such that $d_R(x_i, x_j) \geq 2 \arcsin \sqrt{\delta/N}$ for $i \neq j$. Then,

$$\mathcal{E}(X) \leq m_N + \frac{N^2}{4} D_C(X) \log \frac{N}{2\delta} + \frac{N \log(8\pi\delta)}{4}.$$

So... Small discrepancy plus not too small separation implies small energy.

Relation to other sets of points

A consequence of the last theorem

Corollary

Fix $s \in (0, 2)$. If X_N minimizes the Riesz s -energy

$$\sum_{1 \leq i < j \leq N} \|(X_N)_i - (X_N)_j\|^{-s}$$

for $N \geq 2$, then $\lim_{N \rightarrow \infty} \mathcal{E}(X_N)/m_N = 1$.

This is a reciprocal to a result by P. Leopardi.

Relation to other sets of points

Schiffmann; Sloan, Womersley; Marzo, Ortega–Cerdá, Weymar

Optimal interpolation points: x_j which maximise $\det \phi_i(x_j)$ where ϕ_i form an o.n. basis of spherical harmonics of degree L .

Corollary

For every $L \geq 2$, let $X_{\pi_L} = (x_1, \dots, x_{\pi_L})$ be a set of (non-elliptic) Fekete points. Then

$$\lim_{L \rightarrow \infty} \frac{\mathcal{E}(X_L)}{m_{\pi_L}} = 1.$$

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I do not want to cheat you: this is **not** so good.

The critical set of \mathcal{E}

Laplacian and Maximum Principle

Recall: for $X = (x_1, \dots, x_N) \in \mathbb{S}^N$, where \mathbb{S}^N has the product Riemannian structure,

$$\mathcal{E}(x_1, \dots, x_N) = \log \prod_{i < j} \|x_i - x_j\|^{-1} = - \sum_{i < j} \log \|x_i - x_j\|.$$

Then:

- $\Delta \mathcal{E} = 2N(N - 1)$.

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Then:

- $\Delta \mathcal{E} = 2N(N - 1)$.
- Thus, there exist no local maxima of \mathcal{E} .



The critical set of \mathcal{E}

A concept from game theory

A “Nash equilibrium” is a tuple $X = (x_1, \dots, x_N)$ such that $\mathcal{E}(X)$ cannot be improved if only one of the x_i is moved.

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A “Nash equilibrium” is a tuple $X = (x_1, \dots, x_N)$ such that $\mathcal{E}(X)$ cannot be improved if only one of the x_i is moved.

This is also called a componentwise minimum.

The critical set of \mathcal{E}

A concept from game theory

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This is also called a componentwise minimum.

A corollary from our main result:

Corollary

Let X be a Nash equilibrium of \mathcal{E} . Then,

$$\mathcal{E}(X) < \frac{N^2}{4}. \quad (\text{optimal to the first order term})$$

Elliptic Fekete points and the condition number of polynomials

Shub and Smale's condition number

Let $f : \mathbb{C} \rightarrow \mathbb{C}$ be a polynomial of degree N and let $\zeta \in \mathbb{C}$ be a zero of f . Let

$$\mu(f, \zeta) = \frac{N^{1/2}(1 + \|\zeta\|^2)^{\frac{N-2}{2}}}{|f'(\zeta)|} \|f\|_{B-W}.$$

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This is the *condition number*, which actually controls the sensibility of the zero ζ to perturbations of f . Let

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Theorem (Shub–Smale)

For every polynomial f , we have $\mu(f) \geq 1$. For random f , with probability at least $1/2$ we have $\mu(f) \leq N$.

Elliptic Fekete points and the condition number of polynomials

Best conditioned polynomials.

So, for many polynomials, $\mu(f) \leq N$.

Elliptic Fekete points and the condition number of polynomials

Best conditioned polynomials.

So, for many polynomials, $\mu(f) \leq N$. Can we find one f with that property? **not easy!** even changing N to N^c , c a constant.

Theorem (Shub–Smale)

Let $x_1, \dots, x_N \in \mathbb{S}$ satisfy $\mathcal{E}(X) \leq m_N + c \log N$.

Let $z_1, \dots, z_N \in \mathbb{C}$ be the preimage of x_1, \dots, x_N under the stereographic projection. Let f be the polynomial which has zeros z_1, \dots, z_N .

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$$\mu(f) \leq N^{c+1}.$$

Experiments suggest, for $c = 0$, $\mu(f) \approx \sqrt{N}/2$.

Elliptic Fekete points and the condition number of polynomials

Best conditioned polynomials

What about a reciprocal?

Theorem (B. 2014)

Let $x_1, \dots, x_N \in \mathbb{S}$.

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$$\mathcal{E}(X) \leq \frac{N^2 \log N}{2} + \frac{N^2}{2} \log c + O(N^2) = O(m_N \log N).$$

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$$\mathcal{E}(X) \leq \frac{N^2 \log N}{2} + \frac{N^2}{2} \log c + O(N^2) = O(m_N \log N).$$

Experiments suggest, for $c = 1$, $\mathcal{E}(X) \approx m_N = N^2/4 + \dots$.

Elliptic Fekete points and the condition number of eigenvectors?

Condition numbers for eigenvalue and eigenvector computations

For the eigenvalue it is a classical. For the eigenvector at least since Stewart (1971). Recently revisited by Armentano. Assume $Av = \lambda v$.

$$\kappa_\lambda(A, \lambda, v) = \frac{1}{\text{Angle between right and left eigenvector}}$$

$$\kappa_v(A, \lambda, v) = \|A\|_F \|B^{-1}\|,$$

where $B = \pi_{v^\perp}(A - \lambda I) |_{v^\perp}$

[Armentano 2013]: Geometric context. $\kappa_\lambda \leq \text{constant} \times \kappa_v$.

Elliptic Fekete points and the condition number of eigenvectors?

Computing eigenvectors is polynomial time on the average

Theorem (Armentano, B., Burgisser, Cucker, Shub)

A homotopy algorithm can compute approximations a la Smale of eigenvalues–eigenvectors on Gaussian matrices in average polynomial time $O(n^{7+2c})$, where c is an upper bound on the condition number of the eigenvectors of the initial matrix of the homotopy.

Elliptic Fekete points and the condition number of eigenvectors?

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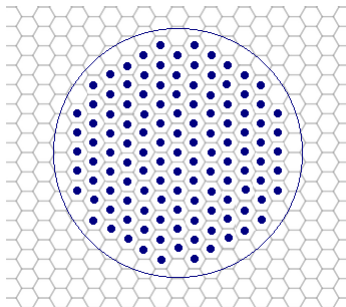
A homotopy algorithm can compute approximations a la Smale of eigenvalues–eigenvectors on Gaussian matrices in average polynomial time $O(n^{7+2c})$, where c is an upper bound on the condition number of the eigenvectors of the initial matrix of the homotopy.

Currently: $c=1$ (next slice) hence average time $O(n^9)$. Can we do better?

Previous result for Hermitian matrices by Armentano and Cucker with randomized algorithm.

Elliptic Fekete points and the condition number of eigenvectors?

A diagonal matrix with optimal condition number

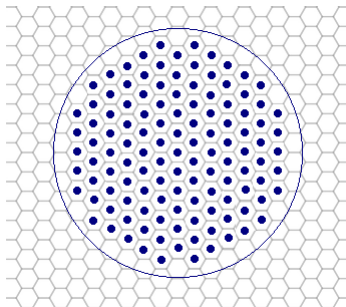


Fix n . Take a radius r enough to put n hexagons of fixed side 1 in the circle of radius r . The diagonal matrix with entries given by the complex coordinates of the blue dots is at most:

$$\frac{n}{\sqrt{6}}.$$

Elliptic Fekete points and the condition number of eigenvectors?

A diagonal matrix with optimal condition number



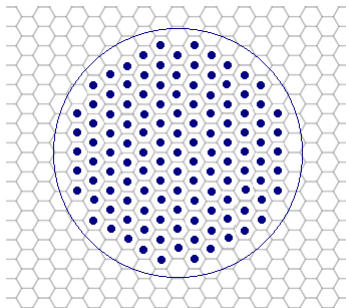
Fix n . Take a radius r enough to put n hexagons of fixed side 1 in the circle of radius r . The diagonal matrix with entries given by the complex coordinates of the blue dots is at most:

$$\frac{n}{\sqrt{6}}.$$

Which is the **actual best**?
Packing problem! Concrete relation to elliptic Fekete points?

Elliptic Fekete points and the condition number of eigenvectors?

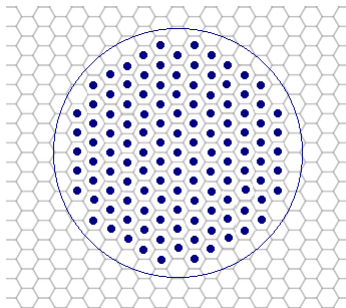
A diagonal matrix with optimal condition number



Does this collection of points solve the original problem by Shub and Smale (find a sequence of well-conditioned polynomials)?

Elliptic Fekete points and the condition number of eigenvectors?

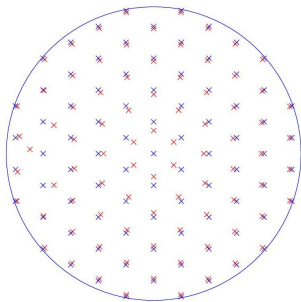
A diagonal matrix with optimal condition number



Does this collection of points solve the original problem by Shub and Smale (find a sequence of well-conditioned polynomials)?
Certainly not: experimentally, the condition number grows as $poly(n)e^n$ where n is the number of points.

Elliptic Fekete points and the condition number of eigenvectors?

A diagonal matrix with optimal condition number



Does this collection of points solve the original problem by Shub and Smale (find a sequence of well-conditioned polynomials)?
Certainly not: experimentally, the condition number grows as $\text{poly}(n)e^n$ where n is the number of points.

Ongoing work

- Understanding the relation between the logarithmic energy and the condition number of polynomials and eigenvectors.
- Investigating the structure of the critical set of \mathcal{E} .
- Juan González Criado del Rey: investigating the topological properties of the set of minimizers of Tammes problem, which might give some insight in the dynamical formation of those pollen grains.

Japanese art and spherical points

Thank you for your attention.

