The Coulomb energy of spherical designs on S^2

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Coulomb energy of a point set on S^2

The Coulomb energy of a point set $X = \{\mathrm{x}_1, \ldots, \mathrm{x}_m\} \subset S^2$, is the energy of the $1/r$ potential on X,

$$E(X) := \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1, j \neq i}^{m} |\mathrm{x}_i - \mathrm{x}_j|^{-1}.$$

On S^2 the potential $|\mathrm{x} - \mathrm{y}|^{-1}$ can also be expressed as

$$|\mathrm{x} - \mathrm{y}|^{-1} = \frac{1}{\sqrt{2 - 2\,\mathrm{x} \cdot \mathrm{y}}}.$$

Key result

For a sequence of point sets on S^2, where

- each set X is a spherical n-design with m points, where $m = O(n^2)$, and where
- the spherical distance between points of X is at least $\lambda/\sqrt{m}$, for some λ common to all sets of the sequence,

the Coulomb energy $E(X)$ is bounded by

$$E(X) \leqslant \frac{1}{2}m^2 + O(m^{3/2}).$$

This bound has the same form as the estimates of the minimum energy of m points on S^2.

Why spherical designs?

If X is a spherical n-design, for the potential $p(\mathrm{x}\cdot\mathrm{y})$, with p a polynomial of degree at most n, the energy is given by

$$\begin{aligned} E(X,p) &= \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1,j\neq i}^{m} p(\mathrm{x}_i\cdot\mathrm{x}_j) \\ &= \frac{1}{2}\frac{m^2}{4\pi}\int_{S^2} p(\mathrm{x}\cdot\mathrm{y})\,ds(\mathrm{x}) - \frac{m}{2}p(1) \\ &= \frac{m^2}{4}\int_{-1}^{1} p(z)\,dz - \frac{m}{2}p(1). \end{aligned}$$

So we split our $1/r$ potential into a polynomial part and a tail, calculate the energy of the polynomial part exactly, and estimate the energy of the tail.

Why have a separation condition?

We want the energy of the tail to be small, so we must keep the points separated.

- The $1/r$ potential is unbounded as $r \longrightarrow 0$, and therefore the tail is also unbounded.
- The disjoint union of two or more spherical n-designs is also a spherical n-design. Call these unions composite spherical n-designs, eg. vertices of two cubes.
- Using composite spherical designs it is easy to construct a sequence where the minimum distance decreases arbitrarily quickly, and the energy increases arbitrarily quickly.
- To exclude such sequences, we must impose a separation condition.

Why use $m^{-1/2}$ in particular?

The sphere is a 2D manifold, so $m^{-1/2}$ is natural.

- The minimum spherical distance is bounded above by

$$\frac{\sqrt{6}}{2}\frac{\pi}{\sqrt{m}}$$

(L. Fejes Tóth, 1949, 1964).

- The minimum energy point sets have minimum spherical distance bounded below by

$$\frac{C}{\sqrt{m}}$$

(Dahlberg, 1978).

Outline of the method

1. Split the potential into a polynomial part of degree n and a tail.

2. Using the properties of the spherical design, calculate the polynomial part of the energy exactly.

3. Use the separation condition to give a bound on the energy contribution of the tail.

Splitting the potential

The identity $(1-z)P_k^{(1,0)}(z) = P_k(z) - P_{k+1}(z)$ leads to a split into a Jacobi partial sum and a well behaved tail, giving

$$\begin{aligned}\frac{1}{\sqrt{2-2t}} &= \sum_{k=0}^{\infty} \frac{2k+2}{(2k+1)(2k+3)} P_k^{(1,0)}(z) \\ &= \sum_{k=0}^{n} \frac{2k+2}{(2k+1)(2k+3)} P_k^{(1,0)}(z) \\ &\quad + \frac{2n+4}{(2n+3)(2n+5)} \frac{P_{n+1}(z)}{1-z} \\ &\quad + \sum_{k=n+2}^{\infty} \frac{2}{(2k-1)(2k+3)} \frac{P_k(z)}{1-z}.\end{aligned}$$

Energy of the polynomial part

For $s_n := \sum_{k=0}^{n} \frac{2k+2}{(2k+1)(2k+3)} P_k^{(1,0)}$ we have

$$E(X, s_n) = \frac{m^2}{4} \int_{-1}^{1} s_n(z)dz - \frac{m}{2} s_n(1)$$

$$= \frac{1}{2}m^2 - \frac{m}{2} \frac{(n+1)(n+2)+m}{2n+3}.$$

If $m = (n+1)^2$ then $E(X, s_n) = \frac{1}{2}m^2 - \frac{1}{2}m^{3/2}$.

Convergence of the tail of the potential

Since $|P_n(z)| \leqslant 1$ for $z \in [-1, 1]$, the series for the tail

$$t_n(z) := \frac{2n+4}{(2n+3)(2n+5)} \frac{P_{n+1}(z)}{1-z} + \sum_{k=n+2}^{\infty} \frac{2}{(2k-1)(2k+3)} \frac{P_k(z)}{1-z}$$

is pointwise absolutely convergent in $[-1, 1)$ and uniformly absolutely convergent in $[-1, 1-\epsilon]$.

Bounding the tail of the potential

From (Bernstein, 1930) we also have, for $0 < \theta < \pi$, $k > 0$,

$$|P_k(\cos\theta)| \leqslant \left(\frac{2}{\pi}\right)^{1/2} k^{-1/2} (\sin\theta)^{-1/2},$$

so for $0 < \theta < \pi$ we have the bound

$$t_n(\cos\theta) \leqslant f(\theta) := \frac{5}{3}\left(\frac{2}{\pi}\right)^{1/2} n^{-3/2} (\sin\theta)^{-5/2},$$

so we also have

$$t_n(-\cos\theta) = t_n(\pi - \theta) \leqslant f(-\theta) = f(\theta).$$

Bounding the energy of the tail

The energy of the tail is given by

$$E(X, t_n) = \frac{1}{2} \sum_{i=1}^{m} E_i(X, t_n),$$

where $$E_i(X, t_n) := \sum_{j=1, j \neq i}^{m} t_n(\mathbf{x}_i \cdot \mathbf{x}_j).$$

For each point $\mathbf{x}_i$, we split S^2 into 4 zones, with $\rho := \frac{\lambda}{2\sqrt{m}}$.

- D_i^+, the closed north polar cap of radius ρ, centre $\mathbf{x}_i$,
- R_i^+, the remainder of the northern hemisphere,
- D_i^-, the closed south polar cap of radius ρ, and
- R_i^-, the remainder of the southern hemisphere.

Bounding the energy of the tail

The tail energy $E_i(X \cap D_i^+, t_n)$ of the north polar cap is zero.

The south polar cap contains at most two points, and $E_i(X \cap D_i^-, t_n) \leqslant 2n^{-1}$.

We estimate the tail energy of $R_i^\pm$ using Riemann-Stieltjes integrals of the form

$$E_i(X \cap R_i^\pm, f) = \int_\rho^{\pi/2} f(\theta) dg_i^\pm(\theta).$$

where $g_i^\pm$ is the counting function corresponding to $X \cap R_i^\pm$.

Counting points

For $\mathbf{x}_i \in X$, $g_i^{\pm}(\theta)$ is the number of points of X in the open spherical collar $S(\pm\mathbf{x}_i, \rho, \theta)$, with centre $\pm\mathbf{x}_i$, inner spherical radius ρ, outer radius θ, where the minimum spherical separation distance is $2\rho = \lambda m^{-1/2}$.

An area argument leads to

$$g_i^{\pm}(\theta) \leqslant \frac{1 - \cos(\theta + \rho)}{1 - \cos\rho}, \quad \text{for} \quad \theta + \rho \leqslant \pi,$$

$$\text{so} \quad g_i^{\pm}(\theta) \leqslant h(\theta) := \frac{\pi^2}{4}\rho^{-2}\sin^2\theta + \pi\rho^{-1}\sin\theta + 1,$$

for $\theta \leqslant \frac{\pi}{2}$. We also know that $g_i^{\pm}(\theta) \leqslant m$.

Bounding the energy of the tail

The Riemann-Stieltjes estimate yields

$$\begin{aligned} E_i(X \cap R_i^{\pm}, f) &= \int_{\rho}^{\pi/2} f(\theta)\, dg_i^{\pm}(\theta) \\ &= f(\pi/2) g_i^{\pm}(\pi/2) - f(\rho) g_i^{\pm}(\rho) - \int_{\rho}^{\pi/2} g_i^{\pm}(\theta)\, df(\theta) \\ &\leqslant f(\pi/2) m - \int_{\rho}^{\pi/2} h(\theta)\, df(\theta) \\ &\leqslant C\lambda^{-5/2} m^{5/4} n^{-3/2}, \end{aligned}$$

so we finally obtain the bound

$$E(X, t_n) \leqslant C_\lambda m^{9/4} n^{-3/2}.$$

Results

Putting the potential back together, we get

$$E(X) \leqslant \frac{1}{2}m^2 - \frac{m}{2}\,\frac{(n+1)(n+2)+m}{2n+3} + C_\lambda m^{9/4} n^{-3/2}$$
$$\leqslant \frac{1}{2}m^2 + O(mn) + O(m^2 n^{-1}) + O(m^{9/4} n^{-3/2}).$$

When $m = O(n^2)$, we have our key result,

$$E(X) \leqslant \frac{1}{2}m^2 + O(m^{3/2}),$$

since $n = O(m^{1/2})$ by the linear programming bound (Delsarte et al., 1977).