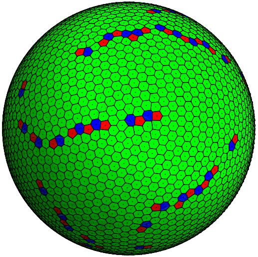
Minimal Discrete Energy on Rectifiable Sets



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Optimal and random point configurations
Institut Henri Poincaré, Paris – June 27 – July 1, 2016

Motivation

Questions from physics

- How does long range order (crystalline structure) arise out of simple pairwise interactions?

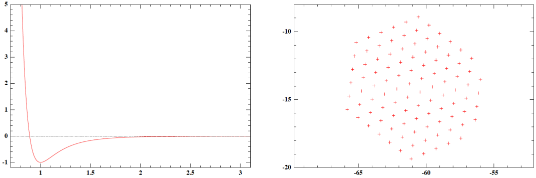


FIGURE 1. Left: the Lennard-Jones potential (3). Right: a minimizer for the variational problem (2), computed numerically in [14], with $N = 100$ and $d = 2$. The particles seem to arrange themselves on an hexagonal lattice, and to form a large cluster having the shape of an hexagon.

Generating good node sets

- Distribute points on a set A according to a given distribution with good local properties.

Figure 1 from X. Blanc, M. Lewin 2015

Discrete energy problem

Let $A \subset \mathbf{R}^p$ be compact with $d = \dim A$ (say $A = \mathbb{S}^d \subset \mathbf{R}^{d+1}$).

For $\omega_N\{\mathbf{x}_1, \ldots \mathbf{x}_N\} \subset A$ and $f : A - A \to \mathbf{R}$, let

$$E_f(\omega_N) := \sum_{i \neq j} f(\mathbf{x}_i - \mathbf{x}_j).$$

DMEP:

$$\mathcal{E}_f(A, N) := \min_{\omega_N \subset A} E_f(\omega_N),$$

Key Examples:

- Reisz potentials $s \neq 0$: $f(\mathbf{x} - \mathbf{y}) := f_s(\mathbf{x} - \mathbf{y}) = \dfrac{\operatorname{sgn}(s)}{|\mathbf{x} - \mathbf{y}|^s}$.
- Log-potential: $f(\mathbf{x} - \mathbf{y}) := f_{\log}(\mathbf{x} - \mathbf{y}) = \log\left(\dfrac{1}{|\mathbf{x} - \mathbf{y}|}\right)$.
- Gaussian $a > 0$: $f(\mathbf{x} - \mathbf{y}) := g_a(\mathbf{x} - \mathbf{y}) = e^{-a|\mathbf{x}-\mathbf{y}|^2}$.

Distributing points on a set: metrics

- Separation:
$$\delta(\omega_N) := \min_{i \neq j} |\mathbf{x}_i - \mathbf{x}_j|$$
- Covering:
$$\rho(\omega_N, A) := \max_{\mathbf{x} \in A} \min_{i} |\mathbf{x} - \mathbf{x}_i|$$
- Maximizing separation $\delta(\omega_N)$: N-**point best-packing** problem on A.
- Minimizing covering radius $\rho(\omega_N, A)$: N-**point best-covering** problem on A.

The limits $a, s \to 0$ and $a, s \to \infty$.

- As $a, s \to \infty$ we recover the best-packing problem on A:

$$\lim_{s\to\infty} E_s(\omega_N)^{1/s} = \lim_{s\to\infty} \left(\sum_{i\neq j} |\mathbf{x}_i - \mathbf{x}_j|^{-s} \right)^{1/s} = \frac{1}{\delta(\omega_N)}$$

$$\lim_{a\to\infty} E_{g_a}(\omega_N)^{1/a} = \lim_{a\to\infty} \left(\sum_{i\neq j} e^{-a|\mathbf{x}_i - \mathbf{x}_j|^2} \right)^{1/a} = e^{-\delta(\omega_N)^2}.$$

- For $r > 0$, we have

$$r^{-s} = 1 + s\log(1/r) + O(s^2) \qquad s \to 0$$
$$e^{-ar^2} = 1 - ar^2 + O(a^2) \qquad a \to 0.$$

Thus:

$$\lim_{s\to 0} \frac{1}{s}\left(E_s(\omega_N) - N(N-1)\right) = E_{\log}(\omega_N)$$
$$\lim_{a\to 0} \frac{1}{a}(E_{g_a}(\omega_N) - N(N-1) = E_{-2}(\omega_N)$$

7 of Smale's 18 Problems for this Century:

Generate $\{x_1, \ldots, x_N\} \subset S^2$ (in polynomial time in N) such that

$$E_{\log}(\{x_1, \ldots, x_N\}) \leq \mathcal{E}_{\log}(S^2, N) + \mathcal{O}(\log N).$$

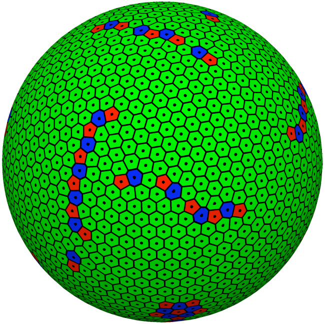


Figure : $N = 1600$ (near) optimal points on S^2 for $s = \log$ energy. Voronoi cells are either pentagons, hexagons, heptagons.

Asymptotics of $\mathcal{E}_{\log}(S^2, N)$

Known:

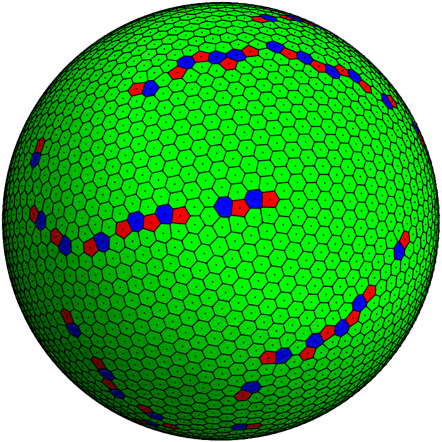
- Wagner (1989):
  $\mathcal{E}_{\log}(S^2, N) = -(1/2)\log(4/e)N^2 - (1/2)N\log N + \mathcal{O}(N)$
- Rakhmanov, Saff, and Zhou (1994):
  $\mathcal{E}_{\log}(S^2, N) = -(1/2)\log(4/e)N^2 - (1/2)N\log N + C_N N$,
  where $-0.2255... < C_N < -0.0469...$ for N sufficiently large.
- Bétermin, Sandier (2016) and Sandier, Serfaty (2015) establish that $C_{\log} := \lim_{N\to\infty} C_N$ exists.

Conjecture:

- Brauchart, Hardin, and Saff (2011):

$$C_{\log} = (1/2)\log(4/e) + \zeta'_{\Lambda_2}(0) = \log\frac{2}{\sqrt{3}} + 3\log\frac{\sqrt{2\pi}}{\Gamma(1/3)} = -0.0556...$$

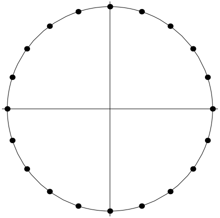
$A = \mathbb{S}^2$, $N = 3000$



3000 points in near minimal $s = 2$-energy configuration on S^2[2]

[2]Show animation. Thanks Alex Vlasiuk and Ken Yang.

The circle $A = \mathbb{S}^1$

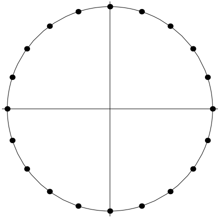


The configuration of equally spaced points $\omega_N = \{e^{i\frac{2\pi k}{N}}\}_{k=1}^{N}$ is optimal for a large class of potentials.

Theorem (Fejes-Tóth, 1956)

Let $f : (0, 2] \to \mathbf{R}$ be decreasing and strictly convex. Then an N-point configuration is an f-energy minimizing configuration if and only if it is equally spaced.

The circle $A = \mathbb{S}^1$



The configuration of equally spaced points $\omega_N = \{e^{i\frac{2\pi k}{N}}\}_{k=1}^N$ is optimal for a large class of potentials.

- For $0 < s \neq 1$,

  $$\mathcal{E}_s(\mathbb{S}^1, N) = V_s N^2 + (2\pi)^{-s} 2\zeta(s) N^{1+s} + O(N^{s-1}), \quad (N \to \infty)$$

  where $\zeta(s)$ is Riemann zeta function and $V_s = \frac{2^{-s}\Gamma((1-s)/2)}{\sqrt{\pi}\Gamma(1-s/2)}$.
- For a complete asymptotic expansion as $N \to \infty$ see [Brauchart, H., Saff, 2011].

$N = 2, 3, d + 2,\ A = \mathbb{S}^d$

Theorem

For $r \in (0, 2]$ let $f(r) = g(r^2)$ for some $g : (0, 4] \to \mathbf{R}$ that is strictly convex and decreasing. A configuration ω_N of $N \leq d + 2$ points is f-energy optimal on $\mathbb{S}^d$ if and only if ω_N is a regular simplex with center at the origin.

Proof.

$N = 2, 3, d+2,\ A = \mathbb{S}^d$

Theorem

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Proof. Consider $\omega_N = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{S}^d$.

$$-E_{-2}(\omega_N) := \sum_{i=1}^{N} \sum_{j \ne i} |\mathbf{x}_i - \mathbf{x}_j|^2 = \sum_{i,j=1}^{N} (2 - 2\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$= 2N^2 - 2 \sum_{i,j=1}^{N} \mathbf{x}_i \cdot \mathbf{x}_j = 2N^2 - 2 \left| \sum_{i=1}^{N} \mathbf{x}_i \right|^2 \le 2N^2,$$

with equality if and only if $\sum_{i=1}^{N} \mathbf{x}_i = \mathbf{0}$.

$N = 2, 3, d+2,\ A = \mathbb{S}^d$

Theorem

For $r \in (0,2]$ let $f(r) = g(r^2)$ for some $g : (0,4] \to \mathbf{R}$ that is strictly convex and decreasing. A configuration ω_N of $N \le d+2$ points is f-energy optimal on $\mathbb{S}^d$ if and only if ω_N is a regular simplex with center at the origin.

Proof. So $-E_{-2}(\omega_N) \le 2N^2$, with "$=$" $\iff \sum_{i=1}^N \mathbf{x}_i = \mathbf{0}$.

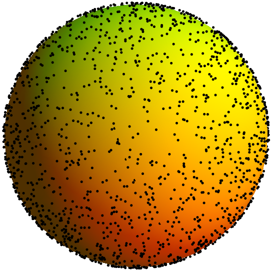
$$E_f(\omega_N) := \sum_{i=1}^{N} \sum_{j:j\neq i} g\left(|\mathbf{x}_i - \mathbf{x}_j|^2\right)$$

$$\ge N(N-1) g\left(\frac{-E_{-2}(\omega_N)}{N(N-1)}\right) \ge N(N-1) g\left(\frac{2N}{N-1}\right)$$

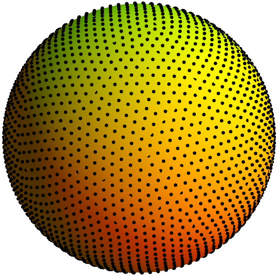
with equality if and only if all pairwise distances $|\mathbf{x}_i - \mathbf{x}_j|$, $i \neq j$, are equal and the configuration has centroid at $\mathbf{0}$.

Random configurations

$\Omega_N = \{X_1, X_2, \ldots X_N\}$: N independent samples chosen according to probability measure μ supported on A.



3000 random points



3000 points near optimal for $s = 2$

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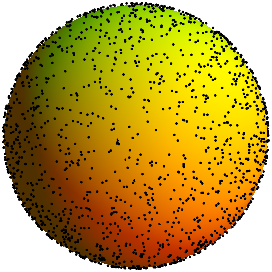

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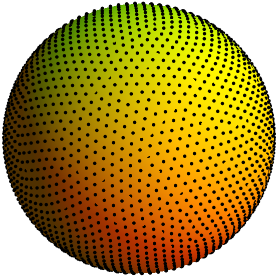

3000 points near optimal for $s = 2$

For recent results on separation and covering of random i.i.d. configurations, see Brauchart, Saff, Sloan, Wang and Womersley, 2016 Saff and Reznikov, 2016.

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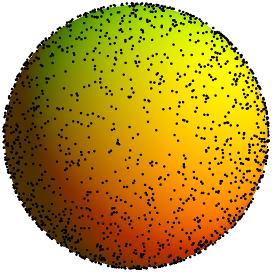

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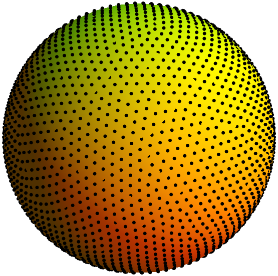

3000 points near optimal for $s = 2$

What about the *s*-energy?

Random configurations

$\Omega_N = \{X_1, X_2, \dots X_N\}$: N independent samples chosen according to probability measure μ supported on A.

$$\mathbb{E}\left[E_s(\Omega_N)\right] = \int \cdots \int \sum_{i \neq j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^s} d\mu(\mathbf{x}_1) \cdots d\mu(\mathbf{x}_N)$$
$$= \sum_{i \neq j} \iint \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^s} d\mu(\mathbf{x}_i) d\mu(\mathbf{x}_j)$$
$$= N(N-1) I_s(\mu)$$

where

$$I_s(\mu) := \iint \frac{1}{|\mathbf{x} - \mathbf{y}|^s} d\mu(\mathbf{x}) d\mu(\mathbf{y}).$$

Equilibrium measure for $s < d$.

Let $A \subset \mathbf{R}^p$ be compact with Hausdorff dimension $d = \dim_{\mathcal{H}}(A)$.

$$\mathfrak{M}_A := \{\text{all Borel probability measures } \mu \text{ on } A\}.$$

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$$I_s(\mu) := \int \int \frac{1}{|x-y|^s} d\mu(y) d\mu(x).$$

- For $s < d$, there exists a unique equilibrium measure μ_s in $\mathfrak{M}_A$ such that

$$I_s(\mu_s) \leq I_s(\mu) \quad \text{for all} \quad \mu \in \mathfrak{M}_A.$$

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$$I_s(\mu_s) \leq I_s(\mu) \quad \text{for all} \quad \mu \in \mathfrak{M}_A.$$

- For $s \geq d$, $I_s(\mu) = \infty$ for all $\mu \in \mathfrak{M}_A$.

Connection Between Continuous & Discrete Problems

Theorem (Polya, Szego, Fekete, Frostman; cf. Landkof)

Let $A \subset \mathbf{R}^p$ *be compact,* $s < d := \dim_{\mathcal{H}}(A)$*, and* μ_s *Riesz s-equilibrium measure on A. Then*

$$\mathcal{E}_s(A, N) = I_s(\mu_s)N^2 + o(N^2), \qquad N \to \infty$$

and minimal s-energy configurations $\omega_N^* = \omega_N^*(A, s)$ *satisfy*[3]

$$\nu_N := \frac{1}{N} \sum_{x \in \omega_N^*} \delta_x \xrightarrow{*} \mu_s \quad as \quad N \to \infty.$$

Recall: If $s < d$ and Ω_N consists of N independent samples of $X \sim \mu_s$ then

$$\mathbb{E}\left[E_s(\Omega_N)\right] = I_s(\mu_s)N(N-1).$$

[3] $\mu_n \xrightarrow{*} \mu$ means $\int f \, d\mu_n \to \int f \, d\mu$ for all $f \in C(A)$.

Proof of Theorem

Step 1: First observe that

$$\mathcal{E}_s(A,N) = E_s(\omega_N^*) = \frac{1}{N-2}\sum_{k=1}^{N} E_s\left(\omega_N^* \setminus \{x_k^*\}\right) \geq \frac{N}{N-2}\mathcal{E}_s(A,N-1).$$

Then

$$\tau_N := \frac{\mathcal{E}_s(A,N)}{N(N-1)} \geq \frac{\mathcal{E}_s(A,N-1)}{N(N-1)}\frac{N}{N-2} = \tau_{N-1}$$

showing that τ_N is **increasing** with N.

Let

$$\tau := \lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N(N-1)}$$

Proof of Theorem

Step 2: Let $\Omega_N = \{X_1, \dots X_N\}$ consist of N independent samples from $X \sim \mu_s$. Then

$$\mathcal{E}_s(A, N) \leq \mathbb{E}(E_s(\Omega_N)) = N(N-1)I_s(\mu_s).$$

Proof of Theorem

Step 2: Let $\Omega_N = \{X_1, \dots X_N\}$ consist of N independent samples from $X \sim \mu_s$. Then

$$\mathcal{E}_s(A, N) \leq \mathbb{E}(E_s(\Omega_N)) = N(N-1)I_s(\mu_s).$$

and so:

$$\tau_N = \frac{\mathcal{E}_s(A, N)}{N(N-1)} \leq I_s(\mu_s) \quad \Rightarrow \quad \tau \leq I_s(\mu_s).$$

Proof of Theorem

Step 3: By weak-star compactness argument (Banach-Alaoglu Thm), ν_N has a weak-star limit pt μ. Consider

$$\begin{aligned}
I_s(\mu) &= \int\int \frac{1}{|x-y|^s} d\mu(x)d\mu(y) \\
&= \lim_{M\to\infty} \int\int \min\left\{\frac{1}{|x-y|^s}, M\right\} d\mu(x)d\mu(y) \\
&= \lim_{M\to\infty} \lim_{N\to\infty} \int\int \min\left\{\frac{1}{|x-y|^s}, M\right\} d\nu_N(x)d\nu_N(y) \\
&\le \lim_{M\to\infty} \lim_{N\to\infty} \frac{1}{N^2}\{\mathcal{E}_s(A,N)+NM\} \\
&= \tau \le I_s(\mu_s).
\end{aligned}$$

So $\mu = \mu_s$ and hence $\tau = I_s(\mu_s)$ and $\nu_N \xrightarrow{*} \mu_s$. □

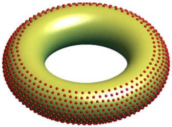
Remarks: General kernel and external field

- The Riesz potential $\frac{1}{|x-y|^s}$ can be replaced by a lower semi-continuous kernel $k(x,y)$ defined on $A \times A$.
- Existence of a unique equilibrium measure requires that there is at least one $\mu \in \mathcal{M}_A$ such that

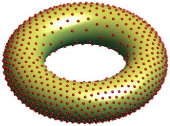
$$I_k(\mu) := \iint k(x,y)\, d\mu(x) d\mu(y) < \infty$$

  and that k is conditionally positive definite: $I_k(\mu) > 0$ for all signed measures μ supported on A such that $I_k(|\mu|) < \infty$ and $\mu(A) = 0$.
- Incorporate an external field $V(x)$ by considering $k_V(x,y) = k(x,y) + (V(x) + V(y))/2$.

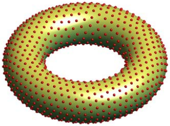
N $= 1000$ **points**



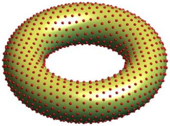
$s = 0.2$



$s = 1.0$

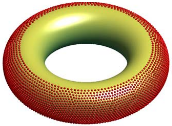


$s = 2.0$

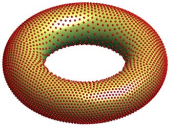


$s = 4.0$

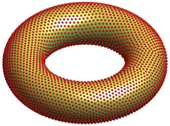
N = 4000 **points**



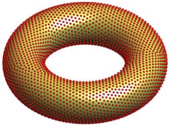
$s = 0.2$



$s = 1.0$

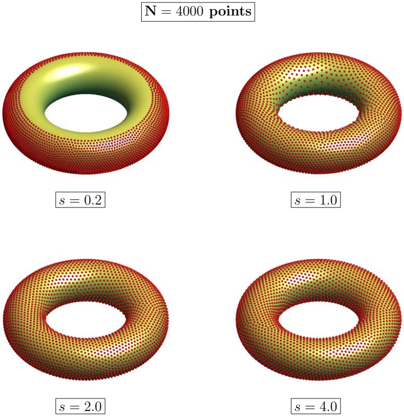


$s = 2.0$



$s = 4.0$

What about bottom two figures ($s = 2, 4$)?



Asymptotics for d-rectifiable sets

A is a **d-rectifiable set** if A is the image of a bounded set in $\mathbf{R}^d$ under a Lipschitz mapping.

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Theorem (H. & Saff, 2005; Borodachov, H. & Saff 2007)

Let A be a compact d-rectifiable set with d-dimensional Hausdorff measure $\mathcal{H}_d(A) > 0$ and suppose $s \geq d$.

- *Optimal s-energy configurations ω_N^* for A have limit distribution uniform wrt $\mathcal{H}_d\big|_A$.*
- *If $s > d$, there exists a constant $C_{s,d}$ (independent of A) such that*

$$\mathcal{E}_s(A, N) = C_{s,d}[\mathcal{H}_d(A)]^{-s/d} N^{1+s/d} + o(N^{1+s/d}).$$

- *Further suppose A is contained in a C^1 d-dimensional manifold then*

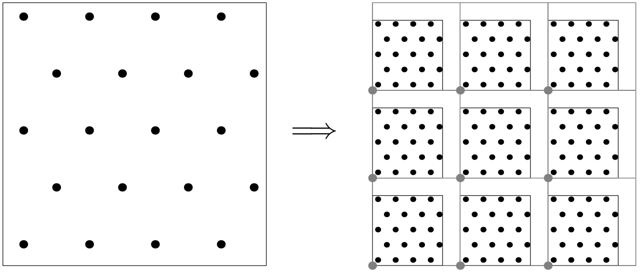
$$\lim_{N\to\infty} \frac{\mathcal{E}_d(A, N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathcal{B}_d)}{\mathcal{H}_d(A)}.$$

Idea of proof.

First establish limit for unit cube $U^d = [0,1]^d$:

$$C_{s,d} := \lim_{N\to\infty} \frac{\mathcal{E}_s(U^d, N)}{N^{1+s/d}}.$$

Key step: The unit cube is self-similar with scaling $1/m$ for any $m = 2, 3, \ldots$. Use this self-similarity to relate $\mathcal{E}_s(A, N)$ and $\mathcal{E}_s(A, m^d N)$. Take $m \to \infty$.



The constant $C_{s,d}$ reflects the 'local' structure of optimal s-energy configurations.

- $C_{s,1} = 2\zeta(s)$ (MMRS, (2005))

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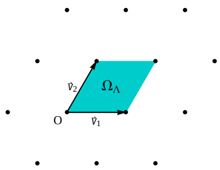
- $C_{s,1} = 2\zeta(s)$ (MMRS, (2005))
- Conjecture (Kuijlaars and Saff, 1998): $C_{s,2} = \zeta_{\Lambda_2}(s)$ for $s > 2$ where Λ_2 denotes the equilateral triangular lattice and, for a d-dimensional lattice Λ,



$$\zeta_\Lambda(s) := \sum_{0 \neq v \in \Lambda} |v|^{-s} \qquad (s > d).$$

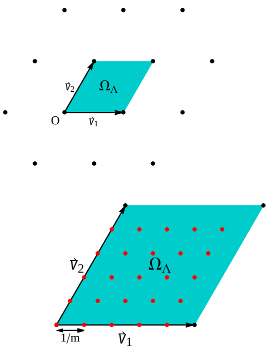
The constant $C_{s,d}$ reflects the 'local' structure of optimal s-energy configurations.

- $C_{s,1} = 2\zeta(s)$ (MMRS, (2005))
- Conjecture (Kuiljaars and Saff, 1998): $C_{s,2} = \zeta_{\Lambda_2}(s)$ for $s > 2$ where Λ_2 denotes the equilateral triangular lattice and, for a d-dimensional lattice Λ,

$$\zeta_\Lambda(s) := \sum_{0 \neq v \in \Lambda} |v|^{-s} \qquad (s > d).$$

- Scaled lattice configurations restricted to a fundamental domain gives:

$$C_{s,d} \leq \zeta_\Lambda(s)|\Lambda|^{-s/d}, \qquad (s > d).$$



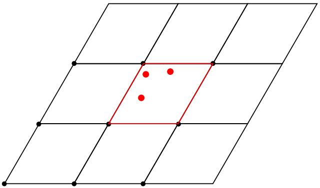
Λ-periodic Riesz energy

- For a lattice $\Lambda \subset \mathbf{R}^d$, $s > d$, and $\omega_N \subset \Omega_\Lambda$ consider

$$E_{s,\Lambda}(\omega_N) := \sum_{x \neq y \in \omega_N} \sum_{v \in \Lambda} \frac{1}{|x - y + v|^s} = \sum_{x \neq y \in \omega_N} \zeta_\Lambda(s; x - y),$$

where

$$\zeta_\Lambda(s; x) := \sum_{v \in \Lambda} \frac{1}{|x + v|^s}, \qquad (s > d, x \in \mathbf{R}^d). \qquad (1)$$



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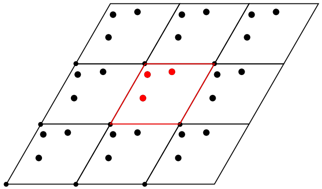

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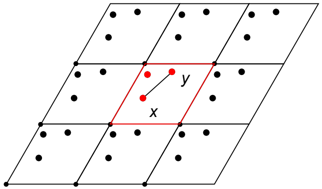

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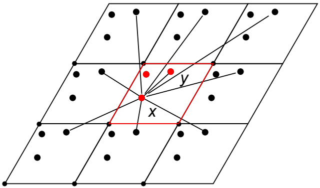

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Theorem (H., Saff, Simanek, 2015)

Let Λ be a lattice in $\mathbf{R}^d$ with co-volume $|\Lambda| > 0$ and $s > d$. Then

$$\lim_{N\to\infty} \frac{\mathcal{E}_{s,\Lambda}(N)}{N^{1+s/d}} = \lim_{N\to\infty} \frac{\mathcal{E}_s(\Omega_\Lambda, N)}{N^{1+s/d}} = C_{s,d}|\Lambda|^{-s/d}, \qquad s > d, \tag{2}$$

$$\lim_{N\to\infty} \frac{\mathcal{E}_{d,\Lambda}(N)}{N^2 \log N} = \lim_{N\to\infty} \frac{\mathcal{E}_d(\Omega_\Lambda, N)}{N^2 \log N} = \frac{2\pi^{d/2}}{d\Gamma(\frac{d}{2})}|\Lambda|^{-1}. \tag{3}$$

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  where

$$\zeta_\Lambda(s; x) := \sum_{v \in \Lambda} \frac{1}{|x + v|^s}, \qquad (s > d, x \in \mathbf{R}^d). \qquad (1)$$

- For $s \leq d$, the sum on the right side of (1) is infinite for all $x \in \mathbf{R}^d$.

Periodizing long range potentials and analytic continuation

- For fixed $x \in \mathbf{R}^d \setminus \Lambda$, it follows (using PSF and Riemann splitting) that $\zeta_\Lambda(s;x)$ has an analytic extension such that

$$F_{s,\Lambda}(x) := \zeta_\Lambda(s;x) + \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{s}{2})(d-s)}, \tag{2}$$

is an entire function.
- We refer to (the analytically extended) $\zeta_\Lambda(s;x)$ as the **Epstein Hurwitz zeta function for the lattice** Λ.

Periodizing long range potentials

For $a > 0$, then

$$F_{s,a,\Lambda}(x) := \sum_{v \in \Lambda} \frac{1}{|x+v|^{-s}} e^{-a|x+v|^2}$$

converges to a finite value for all $x \notin \Lambda$, and there is a C_a such that

$$F_{s,\Lambda}(x) = \zeta_\Lambda(s;x) = \lim_{a \to 0^+} \left(F_{s,a,\Lambda}(x) - C_a \right),$$

so that $E_{s,\Lambda}(\omega_N) := E_{F_{s,\Lambda}}(\omega_N) = \lim_{a \to 0^+} \sum_{x \neq y \in \omega_N} F_{s,a,\Lambda}(x-y).$

Main Result

Theorem (H., Saff, Simanek, Su, 2016)

Let Λ be a lattice in $\mathbf{R}^d$ with co-volume $|\Lambda| > 0$. Then, as $N \to \infty$,

$$\mathcal{E}_{s,\Lambda}(N) = \frac{2\pi^{\frac{d}{2}}|\Lambda|^{-1}}{\Gamma(\frac{s}{2})(d-s)}N^2 + C_{s,d}|\Lambda|^{-s/d}N^{1+\frac{s}{d}} + o(N^{1+\frac{s}{d}}), \qquad 0 < s < d, \tag{3}$$

$$\mathcal{E}_{\log,\Lambda}(N) = \frac{2\pi^{\frac{d}{2}}}{d}|\Lambda|^{-1}N(N-1) - \frac{2}{d}N\log N + \left(C_{\log,d} - 2\zeta_\Lambda'(0)\right)N + o(N). \tag{4}$$

where $C_{\log,d}$ and $C_{s,d}$ are constants independent of Λ.

- Note that the first relation also holds for $s > d$.
- Petrache, Serfaty (2016) establish a result closely related to (**??**) for configurations interacting through a Riesz s potential in an external field for values of the Riesz parameter $d-2 \leq s < d$. Sandier, Serfaty (2015) prove a result closely related to (**??**) for the case that $s = \log$ and $d = 2$.

Universal optimality conjecture for dimensions $d = 2, 4, 8, 24$

- In each of the dimensions $d = 2, 4, 8, 24$, there are special lattices Λ_d, (namely, A_2, D_4, E_8, Leech lattice) that are conjectured by Cohn and Kumar (2007) to be 'universally optimal'; i.e., optimal for energy minimization problems with potentials of the form $f(|x-y|^2)$ for 'completely monotone' f with sufficient decay. If true, then $C_{s,d} = \zeta_{\Lambda_d}(s)$ in these dimensions for $s > 0$ and $s \neq d$.

- Coulangeon and Schürmann (2011) show that such lattice configurations are locally universally optimal under perturbations of both the points and the lattice.
- Optimality for Theta functions (periodized Gaussian potentials)

$$\Theta_{a,\Lambda}(x-y) = \sum_{v\in\Lambda} e^{-a|x-y+v|^2},$$

for all $a > 0$ implies universal optimality.

Connection to Best-Packing

Theorem (BHS)

$$(C_{s,d})^{1/s} \to (1/2)(\beta_d/\triangle_d)^{1/d} \text{ as } s \to \infty,$$

where $\triangle_d$ *is maximal sphere packing density in* $\mathbb{R}^d$ *and* $\beta_d = \mathrm{Vol}(\mathcal{B}^d)$.

$\Delta_1 = 1$,
$\Delta_2 = \pi/\sqrt{12}$ (Thue and Fejes-Toth),
$\Delta_3 = \pi/\sqrt{18}$ (Hales).

The exact value of Δ_d for $d > 3$ is unknown.

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Whoops! (old slide)
$\Delta_8 = \frac{\pi^4}{384}$ (Viazovska, March 14, 2016)
$\Delta_{24} = \frac{\pi^{12}}{12!}$ (Cohn, Kumar, Miller, Radchenko, Viazovska, March 21, 2016)

Cohn & Elkies (2003) provide extremely precise upper bounds for the 'best-packing' density Δ_d in dimensions 2, 8, and 24.

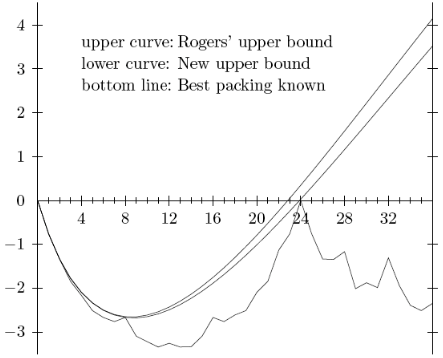

Figure 1. Plot of $\log_2 \delta + n(24-n)/96$ vs. dimension n.

Best packing in dimensions $d = 2$, 8, and 24

Theorem (Cohn, Elkies (2003))

Suppose $f : \mathbf{R}^d \to \mathbf{R}$ *is an admissible function satisfying :*

(1) $f(x) \leq 0$ *for* $|x| \geq r$, *and*

(2) $\hat{f}(t) \geq 0$ *for all* t.

Then $\Delta_d \leq \dfrac{\pi^{d/2}}{(d/2)!} \dfrac{f(0)}{\hat{f}(0)} (r/2)^d$.

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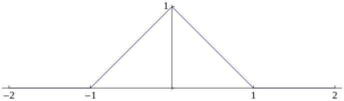
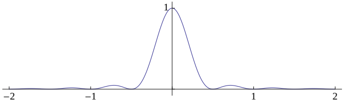
$d = 1$: $\quad f(x) = (1 - |x|)_+ \qquad \hat{f}(t) = \left(\frac{\sin \pi t}{\pi t}\right)^2$





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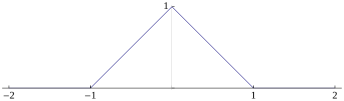

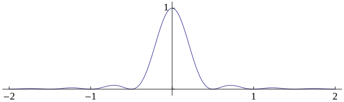

shows $\quad \Delta_1 = \dfrac{\sqrt{\pi}}{(1/2)!} \left(\dfrac{1}{1}\right) (1/2) = 1.$

Prove: $\Delta_d \leq \frac{\pi^{d/2}}{(d/2)!} \frac{f(0)}{\hat{f}(0)} (r/2)^d$

Assume:

- $f(x) \leq 0$ for $|x| \geq r$, and $\hat{f}(t) \geq 0$ for all t.
- $X = \omega_N + \Lambda$ with $\delta(X) = r$.

Note: $\{B(x, r/2)\}_{x \in X}$ forms a sphere packing with density

$$\Delta(X) = \frac{N Vol_d(B(0,1))(r/2)^d}{|\Lambda|} = \frac{\pi^{d/2}}{(d/2)!} \frac{N}{|\Lambda|} (r/2)^d.$$

By PSF

$$\begin{aligned}\sum_{x,y \in \omega_N} \sum_{v \in \Lambda} f(x - y + v) &= \frac{1}{|\Lambda|} \sum_{t \in \Lambda^*} \hat{f}(t) \sum_{x,y \in \omega_N} e^{2\pi i \langle t, (x-y) \rangle} \\ &= \frac{1}{|\Lambda|} \sum_{t \in \Lambda^*} \hat{f}(t) \sum_{x \in \omega_N} \left| e^{2\pi i \langle t, x \rangle} \right|^2\end{aligned}$$

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Since either $x - y + v = 0$ or $|x - y + v| \geq r$ and $\hat{f} \geq 0$,

$$\begin{aligned} Nf(0) &\geq \sum_{x,y \in \omega_N} \sum_{v \in \Lambda} f(x - y + v) \\ &= \frac{1}{|\Lambda|} \sum_{t \in \Lambda^*} \hat{f}(t) \left| \sum_{x \in \omega_N} e^{2\pi i \langle t, x \rangle} \right|^2 \geq N^2 \hat{f}(0), \end{aligned}$$

Thus, $\frac{N}{|\Lambda|} \leq \frac{f(0)}{\hat{f}(0)}$ which gives the result. $\square$

Necessary conditions for optimality

- It is sufficient to consider radial functions.
- To show optimality of lattice Λ, f must vanish on $\Lambda \setminus \{0\}$ and $\hat{f}$ must vanish on $\Lambda^* \setminus \{0\}$.

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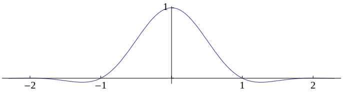
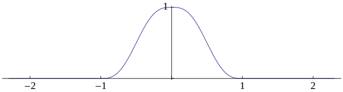
$$f(x) = (1 - x^2) \prod_{k=2}^{\infty} \left(1 - \frac{x^2}{k^2}\right)^2 = \frac{1}{1 - x^2} \left(\frac{\sin \pi x}{\pi x}\right)^2.$$



$$\hat{f}(t) = \left(1 - |t| + \frac{\sin 2\pi|t|}{2\pi}\right) \chi_{[-1,1]}(t)$$



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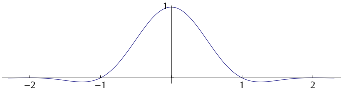

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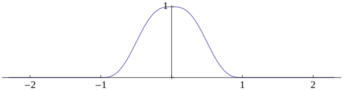

- For $\Lambda = E_8$ or Leech lattice, we have $\Lambda^* = \Lambda$.
- Cohn-Elkies idea: Consider $g_+ = \hat{f} + f$ and $g_- = \hat{f} - f$ which are eigenfunctions of the d-dimensional Fourier transform with eigenvalues 1 or -1, respectively, with "good" double roots.
- Viazovska (March 14) and Cohn et al (March 21) explicitly construct FT-eigenfunctions with eigenvalues ± 1 with double zeros on $\{\sqrt{2n} \mid n = 2, 3, 4, \ldots\}$ using modular forms (Eisenstein series) and then rigorously verify that these can be put combined to give a function f establishing optimality.

Coding Theory Linear Programming Bounds: Notation

- $\mathbb{S}^{n-1}$: unit sphere in $\mathbf{R}^n$
- Spherical Code: A finite set $C \subset \mathbb{S}^{n-1}$ with cardinality $|C|$
- **Interaction potential** $h : [-1, 1] \to \mathbf{R} \cup \{+\infty\}$ (low. semicont.)
- The h-**energy** of a spherical code C:

$$E(n, C; h) := \sum_{x,y \in C, y \neq x} h(\langle x, y \rangle),$$

where $t = \langle x, y \rangle$. Recall $|x - y|^2 = 2 - 2t$.

- Riesz s-potential: $h(t) = (2 - 2t)^{-s/2} = |x - y|^{-s}$
- Log potential: $h(t) = -\log(2 - 2t) = -\log|x - y|$
- hard sphere potential:

$$h(t) = \begin{cases} 0, & -1 \leq t \leq t^* \\ \infty, & t^* \leq t \leq 1 \end{cases}$$

Spherical Harmonics

- $\mathrm{Harm}(k)$: homogeneous harmonic polynomials in n variables of degree k restricted to $\mathbb{S}^{n-1}$ with

$$r_k := \dim \mathrm{Harm}(k) = \binom{k+n-3}{n-2}\left(\frac{2k+n-2}{k}\right).$$

- Spherical harmonics (degree k): $\{Y_{kj}(x) : j = 1, 2, \ldots, r_k\}$ orthonormal basis of $\mathrm{Harm}(k)$ with respect to integration using $(n-1)$-dimensional surface area measure on $\mathbb{S}^{n-1}$.

Gegenbauer polynomials

- Gegenbauer polynomials: For fixed dimension n, $\{P_k^{(n)}(t)\}_{k=0}^{\infty}$ is family of orthogonal polynomials with respect to the weight $(1-t^2)^{(n-3)/2}$ on $[-1,1]$ normalized so that $P_k^{(n)}(1)=1$.
- The Gegenbauer polynomials and spherical harmonics are related through the well-known **Addition Formula**:

$$\frac{1}{r_k}\sum_{j=1}^{r_k} Y_{kj}(x)Y_{kj}(y) = P_k^{(n)}(t), \qquad t=\langle x,y\rangle,\ x,y\in\mathbb{S}^{n-1}.$$

- Consequence: If C is a spherical code of N points on $\mathbb{S}^{n-1}$,

$$\sum_{x,y\in C} P_k^{(n)}(\langle x,y\rangle) = \frac{1}{r_k}\sum_{j=1}^{r_k}\sum_{x\in C}\sum_{y\in C} Y_{kj}(x)Y_{kj}(y)$$

$$= \frac{1}{r_k}\sum_{j=1}^{r_k}\left(\sum_{x\in C} Y_{kj}(x)\right)^2 \geq 0.$$

‘Good’ potentials for lower bounds

Suppose $f : [-1, 1] \to \mathbf{R}$ is of the form

$$f(t) = \sum_{k=0}^{\infty} f_k P_k^{(n)}(t), \qquad f_k \geq 0 \text{ for all } k \geq 1. \tag{5}$$

$f(1) = \sum_{k=0}^{\infty} f_k < \infty \implies$ convergence is absolute and uniform.

Then:

$$\begin{aligned} E(n, C; f) &= \sum_{x,y \in C} f(\langle x, y \rangle) - f(1)N \\ &= \sum_{k=0}^{\infty} f_k \sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) - f(1)N \\ &\geq f_0 N^2 - f(1)N = N^2 \left(f_0 - \frac{f(1)}{N} \right). \end{aligned}$$

Thm (Delsarte-Yudin LP Bound)

Suppose f is of form (**??**) and $h(t) \geq f(t)$ for $t \in [-1, 1]$. Then

$$\mathcal{E}(n, N; h) \geq N^2(f_0 - f(1)/N). \tag{6}$$

An N-point spherical code C satisfies $E(n, C; h) = N^2(f_0 - f(1)/N)$ if and only if both of the following hold:

(a) $f(t) = h(t)$ for all $t \in \{\langle x, y\rangle : x \neq y,\ x, y \in C\}$.

(b) for all $k \geq 1$, either $f_k = 0$ or $\sum_{x,y \in C} P_k^{(n)}(\langle x, y\rangle) = 0$.

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- The **k-th moment** $M_k(C) := \sum_{x,y\in C} P_k^{(n)}(\langle x,y\rangle) = 0$ if and only if $\sum_{x\in C} Y(x) = 0$ for all $Y \in \mathrm{Harm}(k)$.
- If $M_k(C) = 0$ for $1 \leq k \leq \tau$, then C is called a **spherical τ-design** and

$$\int_{\mathbb{S}^{n-1}} p(y)\, d\sigma_n(y) = \frac{1}{N}\sum_{x\in C} p(x), \quad \forall \text{ polys } p \text{ of deg at most } \tau.$$

Thm (Delsarte-Yudin LP Bound)

Suppose f is of form (**??**) and $h(t) \geq f(t)$ for $t \in [-1, 1]$. Then

$$\mathcal{E}(n, N; h) \geq N^2(f_0 - f(1)/N). \tag{6}$$

An N-point spherical code C satisfies $E(n, C; h) = N^2(f_0 - f(1)/N)$ if and only if both of the following hold:

(a) $f(t) = h(t)$ for all $t \in \{\langle x, y\rangle : x \neq y,\ x, y \in C\}$.

(b) for all $k \geq 1$, either $f_k = 0$ or $\sum_{x,y\in C} P_k^{(n)}(\langle x, y\rangle) = 0$.

Maximizing the lower bound (**??**) can be written as maximizing the objective function

$$F(f_0, f_1, \ldots) := N^2\left(f_0 - \frac{1}{N}\sum_{k=0}^{\infty} f_k\right), \qquad (\Delta)$$

subject to (i) $\sum_{k=0}^{\infty} f_k P_k^n(t) \leq h(t)$ and (ii) $f_k \geq 0$ for $k \geq 1$.

Example: n-Simplex on $\mathbb{S}^{n-1}$

Let C be $N = n + 1$ points on $\mathbb{S}^{n-1}$ forming a regular simplex. Then there is only one inner product $\alpha_0 = \langle x, y \rangle$ for $x \neq y \in C$. Since $\sum_{x \in C} x = 0$, it easily follows that $\alpha_0 = -1/n$.

The first degree Gegenbauer polynomial $P_1^{(n)}(t) = t$.

If h is absolutely monotone (or just increasing and convex) then linear interpolant

$$f(t) = h(0) + h'(-1/n)(t + 1/n) = (h(0) + h'(-1/n)/n)P_0^{(n)}(t) + h'(-1/n)P$$

has $f_1 = h'(-1/n) \geq 0$ and, by convexity, stays below $h(t)$ and so shows that the n-simplex is a universally optimal spherical code.

Sharp Codes

Definition

A spherical code $C \subset \mathbb{S}^{n-1}$ is **sharp** if there are m inner products between distinct points in it and C is a spherical $(2m-1)$-design.

Theorem (Cohn and Kumar, 2006)

If $C \subset \mathbb{S}^{n-1}$ is a sharp code, then C is **universally optimal***; i.e., C is h-energy optimal for any h that is absolutely monotone on $[-1,1]$.*

Universal lower bounds for energy

Using results of Levenshtein (1983, 1998) (also the basis of Cohn, Kumar's results) we develop bounds that allow us to solve the linear program restricted to polynomials of certain degrees.

$$D(n,\tau) := \begin{cases} 2\binom{n+k-2}{n-1}, & \text{if } \tau = 2k-1, \\ \binom{n+k-1}{n-1} + \binom{n+k-2}{n-1}, & \text{if } \tau = 2k. \end{cases} \tag{7}$$

$$\tau := \tau(n,N) \quad \text{such that} \quad N \in (D(n,\tau), D(n,\tau+1)]. \tag{8}$$

Levenshtein: there exist quadrature nodes and nonnegative weights

$$-1 \leq \alpha_1 < \cdots < \alpha_k < 1, \quad \rho_1, \ldots, \rho_k \in \mathbb{R}^+, \quad i = 1, \ldots, k \tag{9}$$

such that the Radau/Lobatto $1/N$-quadrature

$$f_0 = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i), \quad \text{for all } f \in \mathcal{P}_\tau. \tag{10}$$

Universal lower bounds for energy

Using results of Levenshtein (1983, 1998) (also the basis of Cohn, Kumar's results) we develop bounds that allow us to solve the linear program restricted to polynomials of certain degrees.

Theorem (Boyvalenkov, Dragnev, H., Saff, Stoyanova, 2016)

*Let n, N be fixed and $h(t)$ be an absolutely monotone potential. Suppose that $\tau = \tau(n,N)$ is as in (**??**), and choose $k = \left\lceil \frac{\tau+1}{2} \right\rceil$. Associate the quadrature nodes and weights α_i and ρ_i, $i = 1, \ldots, k$, as in (**??**). Then*

$$\mathcal{E}(n,N;h) \geq N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i). \tag{7}$$

The Hermite interpolant to h at the nodes α_i solve the linear program (Δ) in Π_τ.

600 cell

- $C = 120$ points in $\mathbf{R}^4$. Each $x \in C$ has 12 nearest neighbors forming an icosahedron (Voronoi cells are dodecahedra).
- 8 inner products between distinct points in C: $\{-1, \pm 1/2, 0, (\pm 1 \pm \sqrt{5})/4\}$.
- 2*7+1 interpolation conditions (would require $\tau = 14$ design)
- C is an 11 design, but almost a 19 design (only 12-th moment is nonzero). I.e. quadrature rule from C is exact on subspace Λ of Π_{19} that is $\perp$ to $P_{12}^{(4)}$.
- Cohn and Kumar find a family of 17-th degree polynomials that proves universal optimality of 600 cell and they require $f_{11} = f_{12} = f_{13} = 0$. Why?

Book to appear in late 2016 (?early 17):

Minimal Energy on Rectifiable Sets

by D. Hardin, E. Saff, and S. Borodachov

Thanks!