Asymptotics of periodic minimal energy problems

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Energy notation

Let A be compact set in $\mathbf{R}^n$ (say $A = \mathbb{S}^{n-1}$)

N-point configuration $\omega_N := \{\mathbf{x}_1, \dots \mathbf{x}_N\} \subset A$

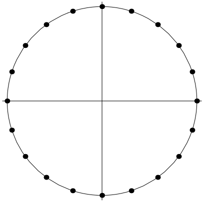
- f-energy:

$$E_f(\omega_N) := \sum_{i=1}^{N} \sum_{j \neq i} f(\mathbf{x}_i - \mathbf{x}_j).$$

- Reisz s-potential: $f_s(\mathbf{x}) := 1/|\mathbf{x}|^s, \quad s > 0.$
- Log-potential: $f_{\log} := \log(1/|\mathbf{x}|).$
- Gaussian: $g_a := e^{-a|x|^2}, \quad a > 0.$
- Minimal Energy Problem: Find describe ω_N^* such that

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

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.

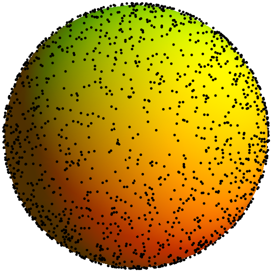
- For $0 < s \neq 1$,

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

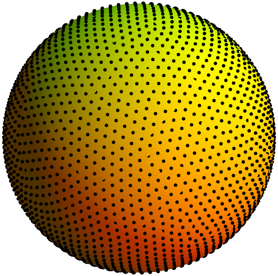
  where $\zeta(s)$ is Riemann zeta function and $V_s = \frac{2^{-s}\Gamma((1-s)/2)}{\sqrt{\pi}\Gamma(1-s/2)}$.
- For a complete asymptotic expansion as $N \to \infty$ see [Brauchart, H., Saff, 2011].

Asymptotics of Random configurations

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



3000 random points



3000 points near optimal for $s = 2$

What about the f-energy?

Asymptotics of Random configurations

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

$$\mathbb{E}\left[E_s(\Omega_N)\right] = \int \cdots \int \sum_{i \neq j} f(\mathbf{x}_i - \mathbf{x}_j) d\mu(\mathbf{x}_1) \cdots d\mu(\mathbf{x}_N)$$

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$$= \sum_{i \neq j} \int \cdots \int f(\mathbf{x}_i - \mathbf{x}_j) d\mu(\mathbf{x}_1) \cdots d\mu(\mathbf{x}_N)$$

$$= \sum_{i \neq j} \iint f(\mathbf{x}_i - \mathbf{x}_j) d\mu(\mathbf{x}_i) d\mu(\mathbf{x}_j)$$

$$= N(N-1) I_s(\mu)$$

where

$$I_s(\mu) := \iint f(\mathbf{x}_i - \mathbf{x}_j) d\mu(\mathbf{x}) d\mu(\mathbf{y}) = \mathbb{E}\left[E_f(\Omega_2)\right].$$

Energy asymptotics for $s < d$ and $s = \log$.

Riesz s-equilibrium measure: $I_s(\mu_s) = \min_{\mu \in \mathcal{P}(A)} I_s(\mu)$

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

Let $A \subset \mathbf{R}^p$ be compact, $s < d := \dim_{\mathcal{H}}(A)$. 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

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

Recall: If $0 < s < d$ and Ω_N consists of N independent samples of $X \sim \mu_s$ then

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

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Conjecture: If $0 < s < d$, there exists a constant $C_{s,d}$ such that

$$\mathcal{E}_s(A, N) = I_s(\mu_s) N^2 + C_{s,d} N^{1+s/d} + o(N^{1+s/d}), \qquad N \to \infty.$$

Energy asymptotics for $s \geq d$.

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

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 satisfy*

$$\nu(\omega_N^*) \xrightarrow{*} (\mathcal{H}_d(A))^{-1}\mathcal{H}_d\big|_A.$$

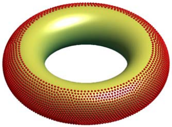
- *If $s > d$, there exists a constant $C_{s,d}$ (independent of A) such that as $N \to \infty$,*

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

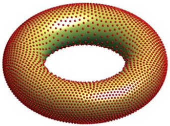
- *if A is also contained in a C^1 d-dimensional manifold then*

$$\mathcal{E}_d(A, N) = (\mathcal{H}_d(\mathcal{B}_d)/\mathcal{H}_d(A))N^2 \log N + o(N^2 \log N).$$

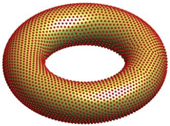
$\mathbf{N} = 4000$ **points**



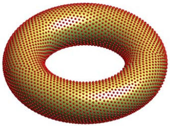
$s = 0.2$



$s = 1.0$



$s = 2.0$



$s = 4.0$

Λ periodic energy

- (Bravais) lattice $\Lambda = A\mathbf{Z}^d$ for some $A \in GL_d(\mathbf{R})$.
- If $f : \mathbf{R}^d \to \mathbf{R}$ decays sufficiently rapidly as $|x| \to \infty$, we consider the Λ periodic potential

$$F_\Lambda(x) := \sum_{v \in \Lambda} f(x+v) = \sum_{v \in \Lambda} f(x-v)$$

- $F_\Lambda(x-y)$ equals energy required to place a unit charge at location $x \in \mathbf{R}^d$ in presence of unit charges at $y + \Lambda = \{y + v : v \in \Lambda\}$.
- F is Λ-periodic, that is, $F(x+v) = F(x)$ for $v \in \Lambda$.
- $\mathcal{E}_F(\mathbf{R}^d, N) = \mathcal{E}_F(\Omega_\Lambda, N)$.

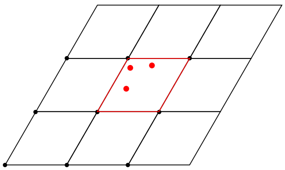
Λ-periodic Riesz energy

- 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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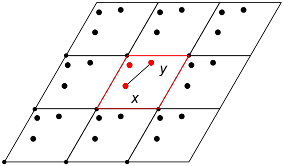

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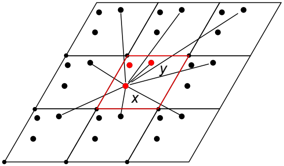

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Theorem (H., Saff, Simanek, 2015)

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

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

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

Λ periodic Riesz s-energy

For $s > d$, the **periodic Riesz s-potential** is

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

and we write

$$\mathcal{E}_{\Lambda,s}(N) := \mathcal{E}_{F_{\Lambda,s}}(\Omega_\Lambda, N).$$

$\zeta_\Lambda(s; x) := F_{\Lambda,s}(x)$ is called the **Epstein-Hurwitz zeta function** for Λ.

Theorem (HSS, 2015)

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

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

where $C_{s,d}$ is the same as in BHS Theorem.

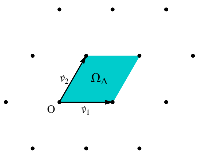
The constant $C_{s,d}$ reflects the 'local' structure of optimal s-energy configurations.

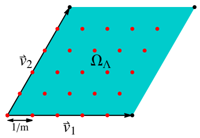
- $C_{s,1} = 2\zeta(s)$ (MMRS, (2005))
- Conjecture (Kuiljaars and Saff, 1998): $C_{s,2} = \zeta_{\Lambda_2}(s)$ for $s > 2$ where Λ_2 denotes the equilateral triangular lattice and, for a d-dimensional lattice Λ,

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

- Scaled lattice configurations restricted to a fundamental domain gives:

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

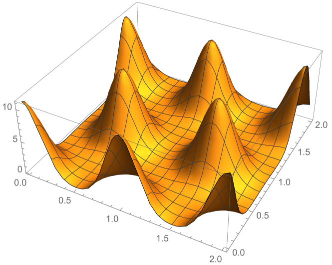




Theta functions: Periodizing Gaussians

- Periodizing $g_a(x-y) = e^{-a|x-y|^2}$, $a > 0$, leads to:

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



- If a configuration ω_N is optimal for $\Theta_\Lambda(a;\cdot)$ for all $a > 0$, then ω_N is Λ-periodic **universally optimal** N-point configuration.

Periodizing long range potentials

- For $s \le d$, the sum $\sum_{v \in \Lambda} \frac{1}{|x-v|^s}$ is infinite for all $x \in \mathbf{R}^d$.
- **convergence factors**: a parametrized family of functions $g_a : \mathbf{R}^d \to [0, \infty)$ such that
  (a) for $a > 0$, $f_s(x) g_a(x)$ has sufficient decay as $|x| \to \infty$ so that

  $$F_{s,a,\Lambda}(x) := \sum_{v \in \Lambda} f_s(x+v) g_a(x+v)$$

  converges to a finite value for all $x \notin \Lambda$, and
  (b) $\lim_{a \to 0^+} g_a(x) = 1$ for all $x \in \mathbf{R}^d \setminus \{0\}$.
- The family of Gaussians $g_a(x) = e^{-a|x|^2}$ is a convergence factor for Riesz potentials. We show that one may choose C_a such that for $0 < s < d$

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

Main Result

Theorem (H., Saff, Simanek, Su, 2017)

Let Λ be a lattice in $\mathbf{R}^d$ with co-volume $|\Lambda| = 1$. Then, as $N \to \infty$,

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

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

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

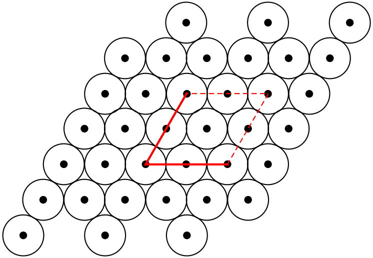
Remark: Petrache and Serfaty (2017) show the existence of related energy limits for $d-2 \leq s < d$ in the context of energy minimizing configurations in the presence of a confining external field.

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

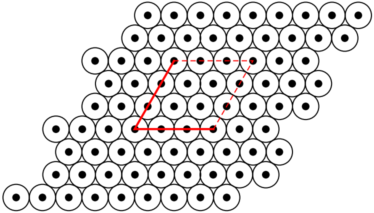
- In each of the dimensions $d = 2, 4, 8, 24$, there are special lattices Λ_d, (namely, A_2, D_4, E_8, Leech lattice) that are conjectured by Cohn and Kumar (2007) to be 'universally optimal'; i.e., optimal for energy minimization problems with potentials F that are periodizations of potentials of the 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 $s \neq d$.

- Cohn, Kumar, Miller, Radchenko, Viazovska, 2020: E_8 and Leech lattice are universally optimal.
- Optimality for Gaussian potentials $g_a(x-y) = e^{-a|x-y|^2}$ (i.e., Theta functions) implies universal optimality.

Optimal N point configurations for Λ_2



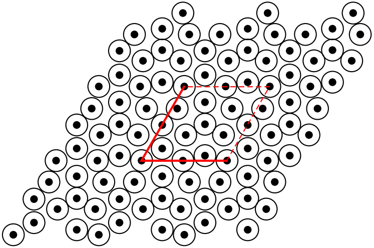
$N = 4$



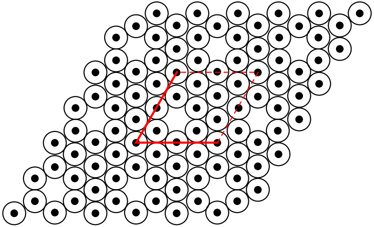
$N = 9$

Conjecture

Let $\Lambda' \subset \Lambda_2$ with co-volume $N \geq 3$ (must be of form $m^2 + mn + n^2$ for $m, n \in \mathbf{Z}$). Then $\omega_N = \Lambda_2 \cap \Omega_{\Lambda'}$ is the unique (up to isometry) universally optimal N-point for appropriate Λ' periodized potentials.



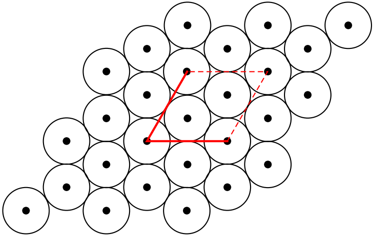
$N = 11, a = 20$



$N = 11, a = 100$

Optimal $N = 2, 3$ point configurations for Λ_2

Y. Su has shown universal optimality for $N = 3$ and $N = 2$.



$N = 3$

Optimal $N = 2, 3$ point configurations for Λ_2

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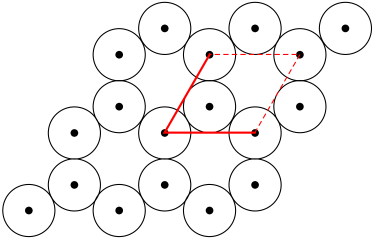

$N = 2$

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