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Discrete Minimum Energy Problems

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Reisz s energy

The Riesz *s*-energy of $\omega_N = \{x_1, x_2, ..., x_N\} \subset \mathbf{R}^{\rho}$ is, for s > 0,

$$E_s(\omega_N) := \sum_{i=1}^N \sum_{j \neq i} k_s(x_i, x_j)$$

where

$$k_s(x,y) := egin{cases} |x-y|^{-s}, & s>0\ -\log\left(|x-y|
ight), & s=0 \end{cases}$$

Note:
$$\frac{|x-y|^{-s}-1}{s} \rightarrow -\log|x-y|$$
 as $s \rightarrow 0$.

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Constrained optimization problem:

Given a compact set $A \subset \mathbf{R}^{p}$.

Minimize the objective function

$$\mathsf{E}_{s}(\omega_{N}) := \sum_{i=1}^{N} \sum_{j \neq i} k_{s}(x_{i}, x_{j})$$

subject to the constraint $\omega_N = \{x_1, \ldots, x_N\} \subset A$.

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subject to the constraint $\omega_N = \{x_1, \ldots, x_N\} \subset A$.

Let $\omega_N^* := \{x_{1,N}, \dots, x_{N,N}\}$ denote an optimal configuration and let $\mathcal{E}_s(A, N) := E(\omega_N^*)$.

Cases s = p - 1 and $s \rightarrow \infty$

The function $k_{p-1}(\cdot, y)$ is harmonic on $\mathbf{R}^p \setminus \{y\}$.



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Cases s = p - 1 and $s \rightarrow \infty$

As $s \to \infty$ and fixed *N*,

$$\left(\sum_{i\neq j}\frac{1}{|x_i-x_j|^s}\right)^{1/s}\rightarrow \frac{1}{\min\{|x_i-x_j|,\ i\neq j\}}$$

Thus, minimal energy configurations become best-packing configurations, i.e., they maximize the minimum pairwise distance between *N* points on *A* as $s \rightarrow \infty$.

Example:
$$A = S^2$$

Describe optimal 2 point configurations.



Example:
$$A = S^2$$

Describe optimal 3 point configurations.



Example:
$$A = S^2$$

Describe optimal 4 point configurations.



Example:
$$A = S^2$$

Describe optimal 5 point configurations.



Example:
$$A = S^2$$

For a configuration of points $\omega_N = \{x_1, \ldots, x_N\} \subset S^2$, let ν_i denote the number of nearest neighbors in ω_N to x_i (i.e., the number of edges for the Voronoi cell for x_i). A simple application of Euler's characteristic formula gives: $\sum_{i=1}^{N} (6 - \nu_i) = 12$.

Best packing in R^d

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Example: $A = S^2$; N = 174; s = 0, 1, 2



Matthew Calef: Vanderbilt PhD student

Example: $A = S^2$; N = 174; s = 0, 1, 2



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Red = heptagon, Green = hexagon, Blue = pentagon



N = 1600, *s* = 4

Best packing in R^d

Spherical crystallography of "colloidosomes"



"Colloidosome" = colloids of radius *a* coating water droplet (radius *R*) -- Weitz Laboratory

Ordering on a sphere \rightarrow a minimum of 12 5-fold disclinations, as in soccer balls and fullerenes -- what happens for R/a >> 1?

- * Adsorb, say, latex spheres onto lipid bilayer vesicles or water droplets
- * Useful for encapsulation of flavors and fragrances, drug delivery
 - [H. Aranda-Espinoza e.t al. Science 285, 394 (1999)]
- *Strength of colloidal 'armor plating' influenced by defects in shell....
- * For water droplets, surface tension prevents buckling....



Confocal image: P. Lipowsky, & A. Bausch

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Questions from physics

- How does long range order (crystalline structure) arise out of simple pairwise interactions?
- How does the structure depend on the geometry of the world *A* (dimension, curvature, ...) in which the particles live. How does the structure depend on the interaction?
- How does the order break down as we move away from the ground state?

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Asymptotics of configurations as $N \rightarrow \infty$

Problem: What is the asymptotic behavior of $\mathcal{E}_s(A, N)$ and of ω_N^* as $N \to \infty$?

- Q1: How are minimal s-energy configurations for A distributed for large N?
- Q2: How does the asymptotic behavior of $\mathcal{E}_s(A, N)$ depend on A and s?

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Connections to Potential Theory

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

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

• For $\mu \in \mathfrak{M}_A$, let

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

• Frostman (1935): For s < d, there exists a unique equilibrium measure μ_s in \mathfrak{M}_A such that

$$I_s(\mu_s) \leq I_s(\nu)$$
 for all $\nu \in \mathfrak{M}_A$

and $I_s(\nu) = \infty$ for $s \ge d$ and all $\nu \in \mathfrak{M}_A$.

- The *s*-capacity of *A* is $cap_s(A) = I_s(\mu_s)^{-1}$.
- Points in an optimal configuration are also called Fekete points.

Connection Between Continuous & Discrete Problems

Theorem (Fekete, 1923; Pólya and Szegő, 1931)

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

$$\lim_{N\to\infty}\frac{\mathcal{E}_{s}(A,N)}{N(N-1)}=I_{s}(\mu_{s})$$

and minimal s-energy configurations $\omega_N^* = \omega_N^*(A, s)$ satisfy in the weak-star topology

$$u_{\mathsf{N}} := \frac{1}{\mathsf{N}} \sum_{x \in \omega_{\mathsf{N}}^*} \delta_x \xrightarrow{*} \mu_s \quad \textit{as} \quad \mathsf{N} \to \infty.$$

Remark: Weak-star convergence of ν_N to μ_s means

$$\frac{1}{N}\sum_{x\in\omega_N^*}^N f(x)\to\int f\,d\mu_s$$

for any $f \in C(A)$.

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Sketch of Proof

Step 1: First observe that

$$\mathcal{E}_{s}(A,N) = E_{s}(\omega_{N}^{*}) = \frac{1}{N-2}\sum_{k=1}^{N}E_{s}(\omega_{N}^{*} \setminus \{x_{k,N}\}) \geq \frac{N}{N-2}\mathcal{E}_{s}(A,N-1).$$

Then

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

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

Let

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

Hypersingular case: $s \ge d$.

Best packing in R^d

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Sketch of Proof

Step 2: Show $\tau \leq I_s(\mu_s)$.

$$\mathcal{E}_{s}(A, N) \leq \sum_{i \neq j}^{N} \frac{1}{|x_{i} - x_{j}|^{s}}, \quad \forall x_{1}, \ldots, x_{N} \in A.$$

$$\mathcal{E}_{s}(A,N) \leq \int_{A} \cdots \int_{A} \sum_{i \neq j}^{N} \frac{1}{|x_{i} - x_{j}|^{s}} d\mu_{s}(x_{1}) \cdots d\mu_{s}(x_{N})$$

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$$\mathcal{E}_s(A, N) \leq \sum_{i \neq j}^N \int_A \int_A \frac{1}{|x_i - x_j|^s} d\mu_s(x_i) d\mu_s(x_j)$$

Best packing in R^d

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eq j}^{N} I_{s}(\mu_{s}) = N(N-1) I_{s}(\mu_{s}) \end{aligned}$$

Hypersingular case: $s \ge d$.

Best packing in R^d

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and so:

$$au_{N} \leq I_{s}(\mu_{s}) \Rightarrow au \leq I_{s}(\mu_{s}).$$

Sketch of Proof

Step 3: By Banach-Alaoglu Thm, ν_N has a weak-star cluster point μ . Consider

$$\begin{split} I_{s}(\mu) &= \int \int \frac{1}{|x-y|^{s}} d\mu(x) d\mu(y) \\ &= \lim_{M \to \infty} \int \int \min\left\{\frac{1}{|x-y|^{s}}, M\right\} d\mu(x) d\mu(y) \\ &= \lim_{M \to \infty} \lim_{N \to \infty} \int \int \min\left\{\frac{1}{|x-y|^{s}}, M\right\} d\nu_{N}(x) d\nu_{N}(y) \\ &\leq \lim_{M \to \infty} \lim_{N \to \infty} \frac{1}{N^{2}} \left\{ \mathcal{E}_{s}(A, N) + NM \right\} \\ &= \tau \leq I_{s}(\mu_{s}). \end{split}$$

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





Surfaces of revolution–the case s = 0

For *A* in the right-half *xy*-plane, let $\Gamma(A)$ denote the set in \mathbb{R}^3 obtained by rotating *A* about the *y*-axis. Let $\mu_{0,Gamma(A)}$ denote the log energy equilibrium on $\Gamma(A)$.



Let A_+ denote the 'right-most' portion of A.

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Surfaces of revolution–the case s = 0

For *A* in the right-half *xy*-plane, let $\Gamma(A)$ denote the set in \mathbb{R}^3 obtained by rotating *A* about the *y*-axis. Let $\mu_{0,Gamma(A)}$ denote the log energy equilibrium on $\Gamma(A)$.



Let A₊ denote the 'right-most' portion of A.

Theorem (H., Saff, and Stahl, 2006)

Suppose A is a compact set in the right-half plane $\mathbb{R}_+ \times \mathbb{R}$. Then the support of the equilibrium measure $\mu_{0,\Gamma(A)}$ is contained in $\Gamma(A_+)$.

J. Brauchart, H., and Saff (2008) also provide related results for 0 < s < 1.



Ed Saff, Vanderbilt



Herbert Stahl, Technische Fachhochschule Berlin





Johann Brauchart, (TU Graz PhD) Vanderbilt



What about $s \ge d$?

For
$$s > d = \dim A$$
, $I_s(\mu) = \infty$ for any $\mu \in \mathfrak{M}_A$. Also

$$\tau = \lim_{N \to \infty} \frac{E_s(A)}{N^2} = \infty.$$

What about $s \ge d$?

For
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$$\tau = \lim_{N \to \infty} \frac{E_s(A)}{N^2} = \infty.$$

So new methods are required for $s \ge d$.

The case $A = S^d$ and s = d.

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The case
$$A = S^d$$
 and $s = d$.

Theorem (Kuijlaars & Saff, 1998)

$$\lim_{N\to\infty} \frac{\mathcal{E}_d(S^d, N)}{N^2 \log N} = \frac{1}{d} \frac{\Gamma((d+1)/2)}{\sqrt{\pi} \, \Gamma(d/2)} = \frac{\operatorname{Vol}(\mathcal{B}_d)}{\operatorname{Area}(S^d)} = \frac{\mathcal{H}_d(\mathcal{B}_d)}{\mathcal{H}_d(S^d)},$$

and (Götz & Saff, 2001) d-energy optimal configurations are asymptotically uniformly distributed on S^d as $N \to \infty$.

Here \mathcal{H}_d denotes *d* dimensional Hausdorff measure on \mathbf{R}^p appropriately normalized.

Grabner and Damelin, 2003, give discrepancy bounds for *d*-energy optimal configurations on S^{d} .

Compact sets in **R**^d

Theorem (H. & Saff, 2005)

Suppose A is a compact set in \mathbf{R}^d . Then

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

(b)
$$\lim_{N \to \infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/d}} = \frac{C_{s,d}}{\left[\mathcal{H}_d(A)\right]^{s/d}}, \ s > d.$$

If $\mathcal{H}_d(A) > 0$, then

$$u_{\mathsf{N}} := rac{1}{\mathsf{N}} \sum_{x \in \omega_{\mathsf{N}}^{*}} \delta_{x} \stackrel{*}{
ightarrow} \mathcal{H}_{\mathsf{d}}^{\mathsf{A}} \quad \textit{as} \quad \mathsf{N}
ightarrow \infty.$$

where $\mathcal{H}_d^A = \frac{\mathcal{H}_d(\cdot \cap A)}{\mathcal{H}_d(A)}$.

About the proof.

An important step in the proof is to show the existence of the limit (2) for $A = U^d := [0, 1]^d$. The unit cube is self-similar with scaling 1/m for any $m = 2, 3, \dots$ We use this to find bounds relating $E_s(A, N)$ and $E_s(A, m^d N)$:



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d-rectifiable sets

 $A \subset \mathbf{R}^{\rho}$ is a *d*-rectifiable set if *A* is the image of a bounded set in \mathbf{R}^{d} under a Lipschitz mapping. If *A* is a *d*-rectifiable set, then *A* is almost the finite disjoint union of almost isometric images of compact sets in \mathbf{R}^{d} :

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d-rectifiable sets

 $A \subset \mathbf{R}^{p}$ is a *d*-rectifiable set if *A* is the image of a bounded set in \mathbf{R}^{d} under a Lipschitz mapping. If *A* is a *d*-rectifiable set, then *A* is almost the finite disjoint union of almost isometric images of compact sets in \mathbf{R}^{d} :

Lemma (Federer, 1969)

If A is a d-rectifiable set then for every $\epsilon > 0$ there exist compact sets $K_1, K_2, K_3, \ldots \subset \mathbf{R}^d$ and bi-Lipschitz mappings $\psi_i : K_i \to \mathbf{R}^\rho$ with constant $1 + \epsilon$, $i = 1, 2, 3, \ldots$, such that $\psi_1(K_1), \psi_2(K_2), \psi_3(K_3), \ldots$ are disjoint subsets of A with

$$\mathcal{H}_d(A\setminus \bigcup_i\psi_i(K_i))=0.$$

Any compact subset of a smooth *d* dimensional manifold is a *d*-rectifiable set.

Minimum energy on *d*-rectifiable sets

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

Suppose $s \ge d$ and $A \subset \mathbf{R}^p$ is a *d*-rectifiable set. When s = d we further assume A is a subset of a *d*-dimensional C^1 manifold. Then

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

(b)
$$\lim_{N \to \infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/d}} = \frac{C_{s,d}}{\left[\mathcal{H}_d(A)\right]^{s/d}}, \ s > d.$$

If $\mathcal{H}_d(A) > 0$, then

$$\nu_{\mathsf{N}} := \frac{1}{\mathsf{N}} \sum_{x \in \omega_{\mathsf{N}}^{*}} \delta_{x} \xrightarrow{*} \frac{\mathcal{H}_{\mathsf{d}}(\cdot)|_{\mathsf{A}}}{\mathcal{H}_{\mathsf{d}}(\mathsf{A})} \quad \textit{as} \quad \mathsf{N} \to \infty.$$

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Problem Definition and Motivation	Potential Theory	Hypersingular case: $s \ge d$.	Best packing in R ^d
The constant $C_{s,d}$			

• d = 1: Since *N*-th roots of unity are optimal on unit circle, we obtain

 $C_{s,1} = 2\zeta(s)$ for s > 1,

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

Summing over lattice configurations gives:

$$C_{s,d} \leq \zeta_d^{\min}(s) := \min_{\Lambda} |\Lambda|^{s/d} \zeta_{\Lambda}(s), \quad s > d.$$
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It is almost surely true (although not proved) that C_{s,2} = |Λ|^{s/d}ζ_Λ(s) where Λ is the equilateral hexagonal lattice. It is conjectured (Cohn and Kumar, 2007) that the E₈ and Leech lattices play the same role in dimensions d = 8 and d = 24.

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Sphere packing density in \mathbf{R}^{d} .

Let \triangle_d denote the largest sphere packing density in \mathbf{R}^d . Connection between $C_{s,d}$ and Δ_d (Borodachov, H., & Saff, 2007)

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$$\Delta_2 = \pi/\sqrt{12} \approx .9069$$
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For d > 3, Δ_d is unknown, although extremely precise bounds are available for d = 2, 8 and 24 (Cohn and Elkies, 2003). Ratio of upper bound to lower bound is

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In each of these dimensions the densest packing appears to be a lattice packing (the hexagonal lattice, E_8 , Leech lattice, respectively).

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

Cohn & Elkies' bounds for Δ_d for d = 2, 8, 24 are based on the following:

Theorem (Cohn & Elkies, 2003)

Suppose $f: {\bf R}^d \to {\bf R}$ is an admissible function satisfying the following three conditions :

(1)
$$f(0) = \hat{f}(0) > 0$$
,

(2)
$$f(x) \le 0$$
 for $|x| \ge r$, and

(3) $\hat{f}(t) \ge 0$ for all *t*.

Then $\Delta_d \leq Vol(B_d)(r/2)^d$.

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Fork in the road

- Fejes Toth's proof of best packing in **R**².
- Movie (Rob Womersley)

Densest packing in R².

The fact that the largest sphere packing $\Delta_2 = \pi/\sqrt{12}$ follows directly from the following:

Theorem (Fejes Toth)

Suppose Ω is a convex polygon in \mathbf{R}^2 with six or fewer sides. Suppose Ω contains N pairwise disjoint open discs of radius r > 0. Then

$$N \leq rac{A(\Omega)}{r^2 a(6)}$$

where $A(\Omega)$ denotes the area of Ω and $a(n) = n \tan(\pi/n)$ denotes the area of the regular n-gon with inradius 1.

Then

$$\frac{N\pi r^2}{A(\Omega)} \leq \frac{\pi}{a(6)} = \pi/\sqrt{12}$$

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Sketch of proof.

Proof.

Let { $B(x_i, r)$ } be a collection of N non-overlapping discs in Ω and let { V_i } denote the Voronoi decomposition of Ω associated with the centers { x_i }^N_{i=1}. Then each V_i is a ν_i -gon containing a disc of radius r.

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