DISCRETE MINIMAL ENERGY PROBLEMS

Lecture II

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Recall Notation

\( \omega_N = \{x_1, \ldots, x_N\} \subset A, \)  \( A \) compact, infinite

\( K : A \times A \rightarrow \mathbb{R} \cup \{+\infty\}, \) symmetric and l.s.c.

\[ E_K(\omega_N) = \sum_{i \neq j} K(x_i, x_j) \]

\[ \mathcal{E}_K(A, N) = \min \{ E_K(\omega_N) : \omega_N \subset A, \#\omega_N = N \} \]

\[ W_K(A) := \min_{\mu \in \mathcal{M}(A)} I_K[A] = \min_{\mu \in \mathcal{M}(A)} \int \int K(x, y) d\mu(x) d\mu(y) \]

\( \mu_A \) equilibrium measure, \( I_K[\mu_A] = W_K(A) \)

\( \nu(\omega_N) = \frac{1}{N} \sum_{x \in \omega_N} \delta_x, \) normalized counting measure
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\[ \nu(\omega_N) = \frac{1}{N} \sum_{x \in \omega_N} \delta_x, \ \text{ normalized counting measure} \]

**Fundamental Thm:** \( \lim_{N \to \infty} \mathcal{E}_K(A, N)/N^2 = W_K(A) \). Every weak* limit measure of the sequence \( \{\nu(\omega^*_N)\}_{N=2}^\infty \) for \( N \)-point \( K \)-energy minimizing configurations \( \omega^*_N \) is an equilibrium measure for the continuous problem on \( A \).
Hereafter $A \subset \mathbb{R}^p$ and $|| \cdot || = |x - y|$, Euclidean distance.

The **Riesz $s$-kernel** is defined by

$$K_s(x, y) := \frac{1}{|x - y|^s}, \quad s > 0; \quad K_{\log}(x, y) := \log \frac{1}{|x - y|}, \quad x, y \in A.$$ 

We write

$$E_s(\omega) := E_{K_s}(\omega), \quad \mathcal{E}_s(A, N) = \mathcal{E}_{K_s}(A, N), \quad s > 0 \text{ or } s = \log.$$ 

For $p = 3$, $s = 1$, get **Coulomb kernel**.

For $A \subset \mathbb{R}^p$ and $s = p - 2$, we get **Newton kernel**.
Some Basic Properties of Riesz Energy

- $A \subset B \Rightarrow \mathcal{E}_s(A, N) \geq \mathcal{E}_s(B, N)$
- $\mathcal{E}_s(A + x, N) = \mathcal{E}_s(A, N)$
- $\mathcal{E}_s(\alpha A, N) = |\alpha|^{-s} \mathcal{E}_s(A, N)$
- $\mathcal{E}_s(A, N)$ is continuous in $s$ for $s > 0$
- $\lim_{s \to 0^+} \frac{\mathcal{E}_s(A, N) - N(N - 1)}{s} = \mathcal{E}_{\log}(A, N)$

and for fixed $N$, every cluster point of minimal $s$-energy $N$-point configurations $\omega_N^{(s)}$ as $s \to 0^+$ is an $N$-point minimal log energy configuration.
Best-Packing and Rieszz Energy ($s \to \infty$)

Recall: Separation distance of $\omega_N = \{x_1, \ldots, x_N\} \subset A$

$$\delta(\omega_N) := \min_{1 \leq i \neq j \leq N} |x_i - x_j|.$$ 

$N$-point best-packing distance on $A$,

$$\delta_N(A) := \sup\{\delta(\omega_N) : \omega_N \subset A, \ #\omega_N = N\},$$

$\omega^*_N$ is best-packing configuration if $\delta(\omega^*_N) = \delta_N(A)$. 

Proposition (Prove it)

For each fixed $N \geq 2$, 

$$\lim_{s \to \infty} E_s(A, N) \frac{1}{s} = \frac{1}{\delta_N(A)}.$$ 

Moreover, every cluster configuration as $s \to \infty$ of $s$-energy minimizing $N$-point configurations on $A$ is an $N$-point best-packing configuration on $A$. 
Best-Packing and Riesz Energy \((s \to \infty)\)

Recall: Separation distance of \(\omega_N = \{x_1, \ldots, x_N\} \subset A\)

\[
\delta(\omega_N) := \min_{1 \leq i \neq j \leq N} |x_i - x_j|.
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\(N\)-point best-packing distance on \(A\),

\[
\delta_N(A) := \sup \{\delta(\omega_N) : \omega_N \subset A, \ #\omega_N = N\},
\]

\(\omega_N^*\) is best-packing configuration if \(\delta(\omega_N^*) = \delta_N(A)\).

**Proposition** (Prove it)

For each fixed \(N \geq 2\),

\[
\lim_{s \to \infty} \mathcal{E}_s(A, N)^{1/s} = \frac{1}{\delta_N(A)}.
\]

Moreover, every cluster configuration as \(s \to \infty\) of \(s\)-energy minimizing \(N\)-point configurations on \(A\) is an \(N\)-point best-packing configuration on \(A\).
Let $A = S^1$, the unit circle in the plane $\mathbb{R}^2$.

Prove that for each $s$, $0 < s < \infty$ or $s = \log$ the $N$-th roots of unity (or any rotation of them) are minimal $s$-energy points for $S^1$. Moreover, they are the only sets of minimal energy points.

More generally: Prove this is true if $K(x, y) = f(|x - y|)$, where $f$ is strictly convex and decreasing on $(0, 2]$. 
\[ S^2 = \{ x \in \mathbb{R}^3 : |x| = 1 \} \]

What about minimal Riesz energy points on \( S^2 \) for

\[ N = 2 \]?
$S^2 = \{ x \in \mathbb{R}^3 : |x| = 1 \}$

What about minimal Riesz energy points on $S^2$ for

$N = 2$ ?

$N = 3$ ?
$S^2 = \{ x \in \mathbb{R}^3 : |x| = 1 \}$

What about minimal Riesz energy points on $S^2$ for

$N = 2$ ?

$N = 3$ ?

$N = 4$ ?
Optimality of Tetrahedron for $S^2 = \{x \in \mathbb{R}^3 : |x| = 1\}$

More generally, for the $d$-dimensional sphere $S^d \subset \mathbb{R}^{d+1}$

**Theorem**

If $K(x, y) = f(|x - y|^2)$, with $f$ strictly convex and decreasing, then for $2 \leq N \leq d + 2$, the only optimal $N$-point $K$-energy configurations on $S^d$ are the vertices of a regular $(N - 1)$-simplex inscribed in $S^d$ centered at 0.
Minimal Riesz $s$-Energy for $N = 5$ on $S^2$
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Bipyramid appears optimal for $s \approx 15$.
Minimal Riesz $s$-Energy for $N = 5$ on $S^2$

**Ratio** of $s$-energy of bipyramid to $s$-energy of optimal sq-base pyramid

Melnyk et al (1977) Bipyramid appears optimal for $0 < s < s^*$ where $s^* \approx 15.04808$.

Recently proved by R. Schwartz (over 150 pages + computer assist).

Open problem for $s > s^* + \epsilon$
MORALS

Optimal Riesz $s$-energy configurations, in general, depend on $s$.

Rigorous proofs of computational observations can be quite difficult.
What do minimal energy points “look like" for large $N$?

What about asymptotics of the minimal energy as $N \to \infty$?
LET’S TALK FOOTBALL (SOCCER)
The Soccer Ball

Vital Statistics
32 faces = 20 hexagons + 12 pentagons
90 edges
60 vertices

Has same structure as Carbon 60 (Bucky Ball)

Question (important for France)
Is it possible to cover (tile) a soccer ball (sphere) with only hexagons?
The Soccer Ball

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France=Le Hexagon
The Soccer Ball

**Euler’s Formula for Convex Polyhedra**

\[ F + V - E = 2. \]

**Examples**

*Cube*: \( 6 + 8 - 12 = 2 \)

*Soccer ball*: \( 32 + 60 - 90 = 2 \)
Assume exactly 3 edges from each vertex.

\( F_5 \) = number of pentagons

\( F_6 \) = number of hexagons

\( F_7 \) = number of heptagons

Then

\[ 3V = 2E \]

\[ 5F_5 + 6F_6 + 7F_7 = 2E \]

So

\[ E = \frac{1}{2}(5F_5 + 6F_6 + 7F_7), \quad V = \frac{1}{3}(5F_5 + 6F_6 + 7F_7) \]

Now let’s apply Euler Formula:
Tiling with 5, 6, and 7-gons

\[ F + V - E = 2 \]

\[ (F_5 + F_6 + F_7) + \frac{1}{3}(5F_5 + 6F_6 + 7F_7) - \frac{1}{2}(5F_5 + 6F_6 + 7F_7) = 2 \]

\[ \frac{1}{6}F_5 + 0F_6 - \frac{1}{6}F_7 = 2 \]

\[ F_5 = F_7 + 12 \]

**Corollary**

If tiling has only hexagons and pentagons, there must be exactly 12 pentagons.

You can’t tile with hexagons alone!
Why is the regular hexagon so important?

For the plane, the hexagon (more precisely, the equilateral triangular lattice) solves the best-packing problem and the best covering problem.

Best-Packing Problem in 2 Dimensions

Arrange nonoverlapping disks all of the same radius in the plane so as to cover the maximal percentage of area.
Why is the regular hexagon so important?

For the plane, the hexagon (more precisely, the equilateral triangular lattice) solves the **best-packing problem** and the **best covering problem**.

**Best-Packing Problem in 2 Dimensions**

Arrange nonoverlapping disks all of the same radius in the plane so as to cover the maximal percentage of area.
Packing disks in 2 dimensions

Proportion of area covered: \[ \frac{\pi}{4} = 0.785... \]

Balls (r=1) per unit area: \[ \frac{1}{4} = 0.25 \]

\[ \frac{2}{\sqrt{3}} \cdot \frac{\pi}{4} = \frac{\pi}{\sqrt{12}} = 0.906... \]

\[ \frac{1}{2\sqrt{3}} = 0.288... \]
Solved by Fejes Toth and also by ...
Solved by Fejes Toth and also by ...
What do minimum energy points for the sphere $S^2$ look like?

Massive high precision experiments were conducted to determine $\mathcal{E}_s(S^2, N)$ for $s = \log$, $s = 1$ and $N = 2, 3, \ldots, 200$.

**Bad News:** There are many local minima of energy that are not global minima. Moreover, the local minima have energies very close to $\mathcal{E}_s(S^2, N)$.

**Good News:** Equilibrium points try to distribute themselves over a nearly spherical hexagonal net.
(Local – Global) Energies $4 \leq N \leq 122$
**Good News:** Equilibrium points try to distribute themselves over a nearly spherical hexagonal net.

\[ N = 122 \text{ electrons in equilibrium (} s = 1 \) \]
Example: 30K ‘minimal’ $s = 3.5$-energy points on $S^2$
Example: 30K ‘minimal’ $s = 3.5$-energy points on $S^2$
Bausch, Bowick, et al

*Grain Boundary Scars and Spherical Crystallography*
Science, March 2003

Model grain boundaries
Spherical crystallography of "colloidosomes"

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

- Adsorb, say, latex spheres onto lipid bilayer vesicles or water droplets
- Useful for encapsulation of flavors and fragrances, drug delivery
  

- Strength of colloidal ‘armor plating’ influenced by defects in shell….
- For water droplets, surface tension prevents buckling….

Ordering on a sphere ➔ a minimum of 12 5-fold disclinations, as in soccer balls and fullerenes -- what happens for \(R/a >> 1\)?
Uniformly distributed spherical configurations

A sequence of $N$-point configurations $\omega_N = \{x_{1,N}, x_{2,N}, \ldots, x_{N,N}\}$, $N = 1, 2, \ldots$ is said to be uniformly distributed on the sphere $S^d$ if

$$\nu(\omega_N) \xrightarrow{*} \sigma_d, \quad N \to \infty,$$

where $\sigma_d$ denotes normalized surface area measure on $S^d$.

Equivalently, for all $f \in C(S^d)$,

$$\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} f(x_{i,N}) = \int_{S^d} f(x) \, d\sigma_d(x).$$
Simple Examples

If $\omega_N = \{e^{2k\pi i/N}\}_{k=0}^{N-1}$, the $N$-th roots of unity, then these configurations are uniformly distributed on the unit circle $S^1$. The normalized counting measures converge weak* to $d\theta/2\pi$, normalized arclength on the unit circle.

Verify that the same is true for the sequence $\{e^{\lambda k\pi i}\}_{k=1}^{\infty}$, whenever $\lambda$ is an irrational real number.
Distributing Points Uniformly on the Sphere

Applications:

- best-packing on sphere
- viral morphology
- crystallography
- electrostatics
- stable molecules (fullerenes)
- data sampling (numerical integration, spherical designs)
- finite normalized tight frames
- testing radar for aircraft
- “soccer” ball designs

Minimizing Riesz energy is one method for generating uniformly distributed points.
3 Classical Problems on $S^2$

- For $s = 1$, get **Thomson’s Problem** for Coulomb potential.
  Answers known for $N = 2, \ldots, 6$ and $12$.

- For $s \to \infty$ with $N$ fixed we get the **Tammes’ Problem**; that is, the best-packing problem.
  Answers known for $N = 2, \ldots, 14$ and $N = 24$.

- For $s = 0$, related to **Smale’s Problem # 7** for 21st century:
  Design polynomial-time algorithm for constructing $\omega_N \subset S^2$ such that
  \[
  E_{\log}(\omega_N) - \varepsilon_{\log}(S^2, N) \leq C \log N, \quad N \geq 2.
  \]
Asymptotics of $\varepsilon_{\log}(S^2, N)$

**Known:**

- Wagner (1989):
  \[ \varepsilon_{\log}(S^2, N) = -(1/2) \log(4/e)N^2 - (1/2)N \log N + O(N) \]

- Rakhmanov, Saff, and Zhou (1994):
  \[ \varepsilon_{\log}(S^2, N) = -(1/2) \log(4/e)N^2 - (1/2)N \log N + C_N N, \]
  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):
  \[ C_{\log} = (1/2) \log(4/e) + \zeta'_2(0) = \log \frac{2}{\sqrt{3}} + 3 \log \frac{\sqrt{2\pi}}{\Gamma(1/3)} = -0.0556... \]
Unit Sphere \( S^d := \{ x \in \mathbb{R}^{d+1} : |x| = 1 \} \)

WHAT’S KNOWN ABOUT LARGE \( N \) ASYMPTOTICS?

For \( 0 < s < d \).

- The Riesz \( s \)-potential of normalized surface area \( \sigma_d \) satisfies
  
  \[
  U^\sigma_d(x) = I_s[\sigma_d] = \frac{\Gamma\left(\frac{d+1}{2}\right)\Gamma(d - s)}{\Gamma\left(\frac{d-s+1}{2}\right)\Gamma(d - s/2)}, \quad x \in S^d.
  \]

- \( K_s(x, y) = \frac{1}{|x - y|^s} \) is strictly positive definite on \( S^d \).
- \( \sigma_d \) is the unique Riesz \( s \)-equilibrium measure.

\[
\lim_{N \to \infty} \frac{\mathcal{E}_s(S^d, N)}{N^2} = W_s(S^d) = I_s[\sigma_d] < \infty,
\]

and any sequence of optimal \( N \)-point \( s \)-energy configurations is asymptotically uniformly distributed on \( S^d \).
What About $s \geq d$?

**Not difficult to show**

$W_s(S^d) = \infty$ for $s \geq d$.

Moreover, for $s > d$, there exist $C_1$, $C_2 > 0$ such that

$$C_1 N^{1+s/d} \leq \mathcal{E}_s(S^d, N) \leq C_2 N^{1+s/d}, \text{ for all } N \geq 2.$$

**Questions:** Does

$$\lim_{N \to \infty} \frac{\mathcal{E}_s(S^d, N)}{N^{1+s/d}} \text{ exist?}$$

What about the limiting distribution of $N$-point minimal $s$-energy configurations?