DISCRETE MINIMAL ENERGY PROBLEMS

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University of Crete, Heraklion May, 2017
Discretizing Surfaces

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Beyond Potential Theory

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Discretizing Surfaces
Beyond Potential Theory
Poppy-Seed Bagel Theorems

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Motivation

Questions from physics

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

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
\[ \omega_N = \{x_1, \ldots, x_N\} \subset A \]

Distributing points on a set: metrics

- **Separation:**
  \[ \delta(\omega_N) := \min_{i \neq j} |x_i - x_j| \]

- **Covering:**
  \[ \rho(\omega_N, A) := \max_{x \in A} \min_{i} |x - x_i| \]

- 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 \( A \).
Best-Packing vs. Best-Covering

Two Trivial Problems:

For $A = [0, 1] \subseteq \mathbb{R}$ solve

Best-packing (maximize min separation)

- - -

Best-covering (minimize largest gap on $A$)

--x--x--x--x--x--x--

Challenge Question:

Same problems for $N = 5$ points, but $[0, 1]$ is replaced by the unit sphere $S^2 \subseteq \mathbb{R}^3$?
Best-Packing vs. Best-Covering

Two Trivial Problems: For $A = [0, 1] \subset \mathbb{R}$ solve

Best-packing (maximize min separation) of 5 points on $A$
Best-Packing vs. Best-Covering

Two Trivial Problems: For $A = [0, 1] \subset \mathbb{R}$ solve

**Best-packing** (maximize min separation) of 5 points on $A$

- $0$  .25  .5  .75  1
Two Trivial Problems: For $A = [0, 1] \subset \mathbb{R}$ solve

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**Best-covering** (minimize largest gap on $A$) for 5 points on $A$
Best-Packing vs. Best-Covering

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- - - - -
0 0.25 0.5 0.75 1

Best-covering (minimize largest gap on $A$) for 5 points on $A$

---x---x---x---x---x---
0.1 0.3 0.5 0.7 0.9
Best-Packing vs. Best-Covering

Two Trivial Problems: For $A = [0, 1] \subset \mathbb{R}$ solve

**Best-packing** (maximize min separation) of 5 points on $A$

![Diagram of points on a line segment]

Best-covering (minimize largest gap on $A$) for 5 points on $A$

![Diagram of points on a line segment with gaps]

Challenge Question: Same problems for $N = 5$ points, but $[0, 1]$ is replaced by the unit sphere $S^2 \subset \mathbb{R}^3$?
Best-packing on $S^2$

200 points in near best-packing on $S^2$
Best-covering on $S^2$

200 points in near best-covering on $S^2$
Let \((A, \| \cdot \|)\) be an infinite compact separable normed linear space. \(K\) a symmetric and lower semi-continuous kernel on \(A \times A\). \(K\)-energy of \(\omega_N = \{x_1, \ldots, x_N\} \subset A\) is

\[
E_K(\omega_N) := \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} K(x_i, x_j) = \sum_{i \neq j} K(x_i, x_j)
\]
Discrete energy

Let \((A, \| \cdot \|)\) be an infinite compact separable normed linear space. \(K\) a symmetric and lower semi-continuous kernel on \(A \times A\). \(K\)-energy of \(\omega_N = \{x_1, \ldots, x_N\} \subset A\) is

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Minimal \(N\)-point \(K\)-energy of the set \(A\) is

\[
\mathcal{E}_K(A, N) := \inf\{E_K(\omega_N) : \omega_N \subset A, \#\omega_N = N\}.
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Discrete energy

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If \(E_K(\omega^*_N) = \mathcal{E}_K(A, N)\), then \(\omega^*_N\) is called \(N\)-point \(K\)-equilibrium configuration for \(A\) or a set of optimal \(K\)-energy points.

In general, \(\omega^*_N\) is not unique.
Continuous Energy Problem

$\mathcal{M}(A)$ is set of all probability measures with support on $A$. $K(x, y)$ symmetric, nonnegative, and l.s.c. kernel on $A \times A$. 
Continuous Energy Problem

\[ \mathcal{M}(A) \] is set of all probability measures with support on \( A \).
\[ K(x, y) \] symmetric, nonnegative, and l.s.c. kernel on \( A \times A \).

**Continuous energy** of \( \mu \in \mathcal{M}(A) \) is defined by

\[
I_K[\mu] := \int\int_{A \times A} K(x, y) \, d\mu(x) \, d\mu(y).
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**Wiener constant** is defined as

\[
W_K(A) := \min\{I_K[\mu] : \mu \in \mathcal{M}(A)\}.
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Continuous Energy Problem

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**Equilibrium measure** is a measure \( \mu_A \in \mathcal{M}(A) \) such that

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If \( W_K(A) = \infty \), (i.e. \( \text{cap}_K(A) := 1/W_K(A) = 0 \)), then every \( \mu \in \mathcal{M}(A) \) is an equilibrium measure.
We say that a sequence of measures \((\mu_n)\) in \(\mathcal{M}(A)\) converges \textbf{weak-star} to a measure \(\mu \in \mathcal{M}(A)\) if for all \(f \in C(A)\)

\[
\lim_{n \to \infty} \int f \, d\mu_n = \int f \, d\mu,
\]

and we write \(\mu_n \xrightarrow{\ast} \mu\).

**Proposition**

If \(\mu_n \xrightarrow{\ast} \mu\) in \(\mathcal{M}(A)\) and \(g\) is l.s.c on \(A\), then

\[
\int g \, d\mu \leq \liminf_{n \to \infty} \int g \, d\mu_n.
\]
Existence of Equilibrium Measure

$K(x, y)$ symmetric, l.s.c. on $A \times A$, where $A$ is compact,

$K$-potential

$$U_K^\mu(x) := \int K(x, y) d\mu(y), \quad \mu \in \mathcal{M}(A)$$

Principle of Descent

If

$$\mu_n \in \mathcal{M}(A), \quad \mu_n \overset{*}{\rightarrow} \mu,$$

then

$$U_K^\mu(x) \leq \liminf_{n \rightarrow \infty} U_K^{\mu_n}(x), \quad x \in A$$

and

$$I_K[\mu] \leq \liminf_{n \rightarrow \infty} I[\mu_n].$$

$U_K^\mu$ and $I_K[\mu]$ are l.s.c. on $\mathcal{M}(A)$, so $I_K[\mu]$ attains its min on $\mathcal{M}(A)$. 
Connection between discrete and continuous energy

**Fundamental Theorem** (Frostman, Choquet, Fekete, Szegő,...)

With $K$ as above,

$$\lim_{N \to \infty} \frac{\varepsilon_K(A, N)}{N^2} = W_K(A).$$

Moreover, if $(\omega^*_N)$ is any sequence of $N$-point $K$-energy minimizing configurations on $A$, then every weak* limit measure $\lambda$ as $N \to \infty$ of the normalized counting measures

$$\nu(\omega^*_N) := \frac{1}{N} \sum_{x \in \omega^*_N} \delta_x$$

is an equilibrium measure for the continuous energy problem on $A$; i.e., $I_K[\lambda] = W_K(A)$. 
Proof of Fundamental Theorem

**Step 1:** Show that \( \frac{E_K(A, N)}{N(N-1)} \) is increasing with \( N \). Set

\[
\tau_K(A) := \lim_{N \to \infty} \frac{E_s(A, N)}{N^2},
\]

which is called the **\( K \)-transfinite diameter** of \( A \).

**Step 2:** Show that \( \tau_K(A) \leq W_K(A) \).

**Step 3:** Prove that \( \tau_K(A) \geq W_K(A) \) and that any weak* limit measure of normalized counting measures associated with a sequence of optimal \( N \)-point \( K \)-energy configurations is an equilibrium measure for the continuous problem.
Uniqueness of equilibrium measures

Let \( \mu \) and \( \nu \) be two finite positive Borel measures on \( A \). Their mutual \( K \)-energy is

\[
\langle \mu, \nu \rangle_K := \iint_{A \times A} K(x, y) \, d\mu(x) \, d\nu(y).
\]

If \( \mu \) and \( \nu \) are finite signed measures we write \( \mu = \mu^+ - \mu^- \) and \( \nu = \nu^+ - \nu^- \) and set

\[
\langle \mu, \nu \rangle_K := \langle \mu^+, \nu^+ \rangle_K + \langle \mu^-, \nu^- \rangle_K - \langle \mu^+, \nu^- \rangle_K - \langle \mu^-, \nu^+ \rangle_K
\]

whenever well-defined.

Definition

A kernel \( K \) on \( A \times A \) is strictly positive definite if for any finite signed measure \( \nu \) for which \( \langle \nu, \nu \rangle_K \) is well-defined, we have \( \langle \nu, \nu \rangle_K \geq 0 \) with equality iff \( \nu = 0 \).
Uniqueness of equilibrium measures

**Lemma**

Let $K$ be symmetric, l.s.c. and **strictly positive definite** on $A \times A$. If $\mu_1, \mu_2 \in \mathcal{M}(A)$ have finite $K$-energies, then

$$\langle \mu_1, \mu_2 \rangle_K \leq \frac{1}{2} (I_K[\mu_1] + I_K[\mu_2])$$

with equality iff $\mu_1 = \mu_2$.

**Theorem**

If $K$ is as above and $W_K(A) < \infty$ that is, $\text{cap}_K(A) > 0$, then the equilibrium measure $\mu_A$ is unique.
One (lucky) way to find equilibrium measure:

**Corollary**

Let $K$ be symmetric, l.s.c. and **strictly positive definite** on $A \times A$. If $\mu \in \mathcal{M}(A)$ is a measure such that $U_K^\mu(x)$ is identically constant on $A$, then $\mu = \mu_A$. 