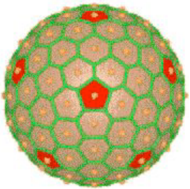
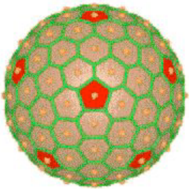


DISCRETE MINIMAL ENERGY PROBLEMS

E. B. Saff
Center for Constructive Approximation
Vanderbilt University

University of Crete, Heraklion May, 2017



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Discretizing Surfaces

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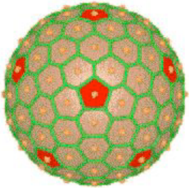

DISCRETE MINIMAL ENERGY PROBLEMS

Discretizing Surfaces
Beyond Potential Theory

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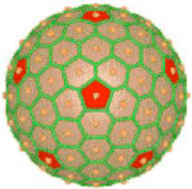

DISCRETE MINIMAL ENERGY PROBLEMS

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?

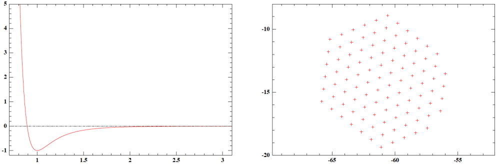

FIGURE 1. Left: the Lennard-Jones potential (3). Right: a minimizer for the variational problem (2), computed numerically in [14], with $N = 100$ and $d = 2$. The particles seem to arrange themselves on an hexagonal lattice, and to form a large cluster having the shape of an hexagon.

Generating good node sets

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

$$\omega_N = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset A$$

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.

Best-Packing vs. Best-Covering

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

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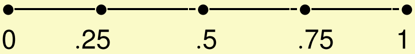

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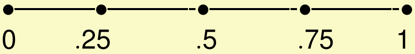

Best-covering (minimize largest gap on A) for 5 points on A

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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

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

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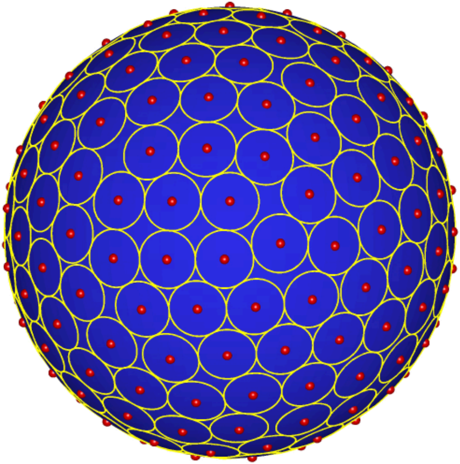
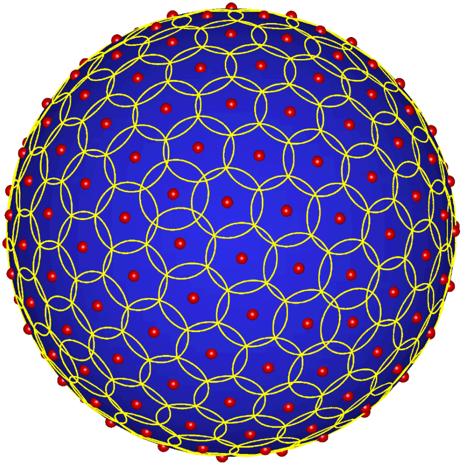
Challenge Question: Same problems for $N = 5$ points, but $[0, 1]$ is replaced by the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$?

Best-packing on $\mathbb{S}^2$



200 points in near best-packing on $\mathbb{S}^2$

Best-covering on $\mathbb{S}^2$



200 points in near best-covering on $\mathbb{S}^2$

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

$$E_K(\omega_N) := \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} K(x_i, x_j) = \sum_{i \neq j} K(x_i, x_j)$$

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If $E_K(\omega_N^*) = \mathcal{E}_K(A, N)$, then ω_N^* is called N-point K-equilibrium configuration for A or a set of optimal K-energy points.
In general, ω_N^* is not unique.

Continuous Energy Problem

$\mathcal{M}(A)$ is set of all probability measures with support on A.
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If $W_K(A) = \infty$, (i.e. $\mathrm{cap}_K(A) := 1/W_K(A) = 0$), then every $\mu \in \mathcal{M}(A)$ is an equilibrium measure.

Existence: Weak* convergence of measures

We say that a sequence of measures (μ_n) in $\mathcal{M}(A)$ converges **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 $\mu_n \xrightarrow{*} \mu$.

Proposition

If $\mu_n \xrightarrow{*} \mu$ 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**

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

Principle of Descent

If

$$\mu_n \in \mathcal{M}(A), \; \mu_n \xrightarrow{*} \mu,$$

then

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

and

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

U_K^{μ} 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,

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

Moreover, if (ω_N^*) is any sequence of N-point K-energy minimizing configurations on A, then every weak* limit measure λ 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 $\frac{\mathcal{E}_K(A,N)}{N(N-1)}$ is **increasing** with N. Set

$$\tau_K(A) := \lim_{N\to\infty} \frac{\mathcal{E}_s(A,N)}{N^2},$$

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 μ and ν be two finite positive Borel measures on A. Their **mutual K-energy** is

$$\langle \mu, \nu \rangle_K := \iint\limits_{A\times A} K(x,y)\, d\mu(x) d\nu(y).$$

If μ and ν 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 ν 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

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

with equality iff $\mu_1 = \mu_2$.

Theorem

If K is as above and $W_K(A) < \infty$ that is, $\mathrm{cap}_K(A) > 0$, then the equilibrium measure μ_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 $\mu = \mu_A$.