Asymptotic properties of short-range interaction functionals

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A tale of two problems

- Optimal quantization

$$\inf_{f \in \mathcal{F}_N} \mathbb{E}\|\xi - f(\xi)\|^p$$

N-quantization error for the random variable ξ
$\mathcal{F}_N$ – functions taking at most N values in $\mathbb{R}^d$

Example:

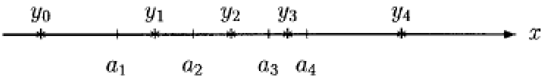


Figure: Quantization scheme with the quantizer $f(x) = \sum_i y_i 1_{S_i}(x)$ (from Gray-Neuhoff)

Equivalently,

$$\inf_{\omega_N \subset \mathbb{R}^d} M_N^p(\omega_N, \mu_\xi)$$

for

$$M_N^p(\omega_N, \mu_\xi) = \int \min_{y_i \in \omega_N} \|x - y_i\|^p \, d\mu_\xi(x)$$

Optimal quantization I

Yet another formulation (as in Stefan's talk):

$$\inf_{\nu \in \mathcal{P}_N} W_p(\mu, \nu)^p = \inf_{\omega_N \subset \mathbb{R}^d} M_N^p(\omega_N, \mu_\xi)$$

with

$$W_p(\mu, \nu) := \inf_{\pi \in \Pi} \left(\int_{\mathbb{R}^d} \|x - y\|^p \, d\pi(x, y) \right)^{1/p},$$

$\mu(x), \nu(y)$ are the marginals of $\pi(x, y)$
$\mathcal{P}_N$ – probability measures supported on at most N points

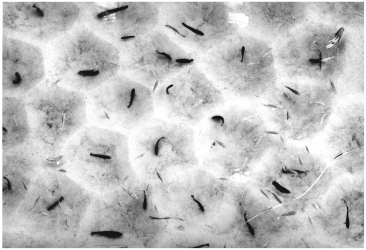
Optimal quantization II

- Introduced as a problem of signal compression by Oliver-Pierce-Shannon (1948)
- Information theory community (Zador, Bucklew-Wise) in the 80s
- Asymptotic properties for $N \to \infty$ studied: under the assumption $\mathbb{E}\|\xi\|^{p+\delta} < \infty$, and $h = \frac{d\mu_\xi}{d\lambda_d}$,

$$\lim_{N\to\infty} N^{p/d} \min_{\omega_N} M_N^p(\omega_N, \mu_\xi) = c_{p,d} \left(\int h^{d/(p+d)} \, d\lambda_d \right)^{(p+d)/d}$$

  with the optimal quantizers converging to $h^{d/(p+d)}$, normalized.
- Most general form due to Gruber (2004)

▶ Applications to generating distributions in the 90s (Lloyd's algorithm; Du-Faber-Gunzburger)



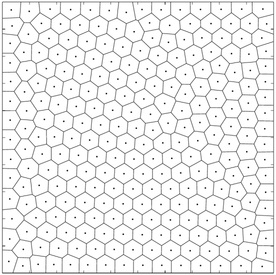


Figure: Left: A top-view photograph, using a polarizing filter, of the territories of the male *Tilapia mossambica*; each is a pit dug in the sand by its occupant. The boundaries of the territories, the rims of the pits, form a pattern of polygons. Photograph and caption from G. W. Barlow, *Hexagonal Territories*, Animal Behavior, Volume 22, 1974.
Right: Centroidal Voronoi tessellation of the unit square (from Du-Faber-Gunzburger).

Hypersingular Riesz interactions I

- Measure μ minimizing the interaction functional

$$\mu \mapsto \int_A \|x-y\|^{-s} \, d\mu(x)d\mu(y), \qquad 0 < s < d, \quad A \subset \mathbb{R}^d$$

  for a fixed domain A is not easy to determine ($s = d-2$ gives harmonic measure)
- For $s > d$ (*hypersingular case*), the continuous problem cannot be formulated as above, but the discrete problem still can be considered:

$$E_s(\omega_N; \eta) = \sum_i \sum_{j \neq i} \eta(x_i) \|x_i - x_j\|^{-s}$$

Hypersingular Riesz interactions II

- Hardin-Saff (2004), Hardin-Saff-Borodachov (2008) study the asymptotic properties for $N \to \infty$ of the discrete problem, showing

$$\lim_{N\to\infty} \frac{\min_{\omega_N \subset A} E_s(\omega_N;\eta)}{N^{1+s/d}} = C_{s,d} \left(\int_A \eta^{-d/s} \, d\lambda_d \right)^{-s/d}$$

with the optimal configurations converging to $h^{-d/s}$, normalized.

- Hardin-Saff-V (2017) computes the distribution for the hypersingular Riesz with external field,

$$E_s(\omega_N; 1, V) = \sum_i \sum_{j\neq i} \|x_i - x_j\|^{-s} + N^{s/d} \sum_i V(x_i)$$

- Applications to generating point distributions

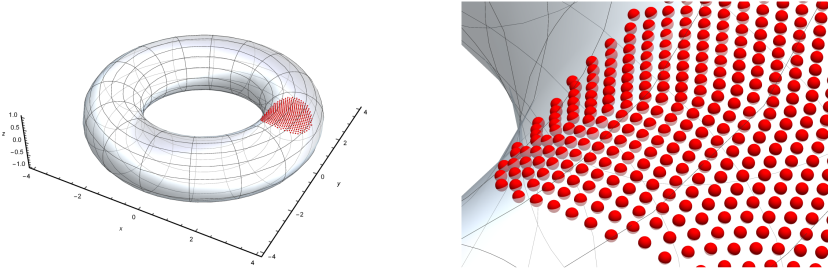


Figure: Approximate optimizers for the hypersingular Riesz interaction with an external field.

k-nearest neighbor Riesz interactions

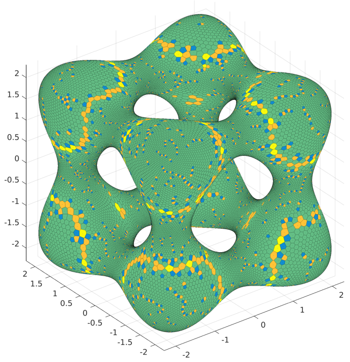
- Many physical models with nearest-neighbor interactions
- The same asymptotic results hold for the Riesz interaction truncated to several nearest neighbors:

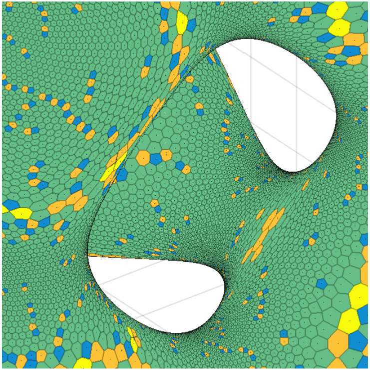
$$E_s^k(\omega_N;\eta) = \sum_{i=1}^{N} \sum_{j \in I_{i,k}} \eta(x_i) \|x_i - x_j\|^{-s}, \qquad s > 0,$$

  where $I_{i,k}$ = the set of indices of k nearest neighbors of x_i in ω_N, ordered by nondecreasing distance to x_i; k fixed.
- Namely,

$$\lim_{N\to\infty} \frac{\min_{\omega_N \subset A} E_s^k(\omega_N;\eta)}{N^{1+s/d}} = C_{s,d}^k \left(\int_A \eta^{-d/s}\, d\lambda_d \right)^{-s/d}$$

Figure: Approximate minimizer of E_s^k on a surface.





Question

What is common to the above problems?

- The limiting distribution can be determined.
- The unweighted interaction is scale-invariant and translation-invariant.
- Remote parts of ω_N do not interact much.

Short-range interactions

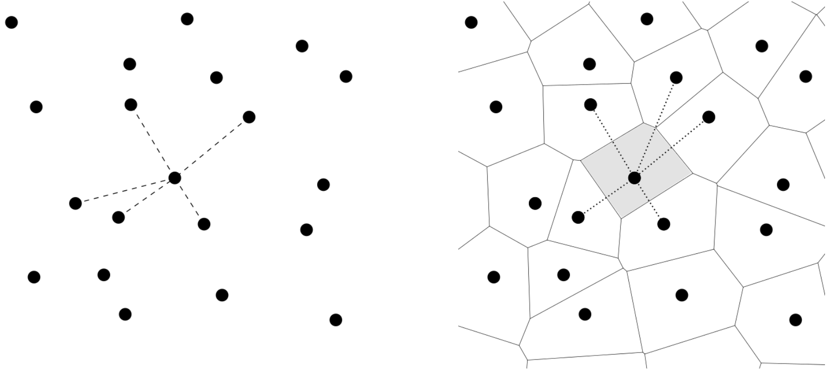


Figure: Left: truncated Riesz energy only includes terms for k nearest neighbors of every $x \in \omega_N$. Right: quadratic quantization error depends on the second moment of Voronoi cells of such x, the shape of which depends on the position of points with adjacent cells only. Both interactions are short-range.

Interactions

- Functionals of the form

$$\mathfrak{e}(\cdot\, A) : \omega_N \to [E_0, \infty], \qquad \omega_N \subset \mathbb{R}^d,\ N \geqslant N_0(\mathfrak{e}), \quad A \subset \Omega$$

  optimized by $\omega_N^*(A)$ on A.
- We study the asymptotics:

$$\mathfrak{L}_{\mathfrak{e}}(A) := \lim_{N\to\infty} \frac{\mathfrak{e}(\omega_N^*(A))}{\mathfrak{t}(N)}, \qquad A \subset \mathbb{R}^d,\ \text{compact}.$$

- Semicontinuous in ω_N, monotonic in A:

$$\operatorname{sgn}\sigma \cdot \mathfrak{L}_{\mathfrak{e}}(A) \geqslant \operatorname{sgn}\sigma \cdot \mathfrak{L}_{\mathfrak{e}}(B) \qquad \text{for} \quad A \subset B,$$

Asymptotics of interaction functionals

Theorem (Hardin-Saff-V, 2020+)

Take $\mathfrak{e}$ *as above, suppose the rate* $\mathfrak{t}(N)$ *is monotonic and* $\lim_{N\to\infty} \mathfrak{t}(tN)/\mathfrak{t}(N) = \mathfrak{w}(t)$ *for a strictly convex* $\mathfrak{w}$*, and any* $t > 0$*. If*

(a) $0 < \mathfrak{L}_{\mathfrak{e}}(x + a\boldsymbol{q}_d) < +\infty$ *exists for any* $x + a\boldsymbol{q}_d \subset \Omega$ *and depends on* a*, not* x*;*

(b) $\mathfrak{e}$ *is short-range;*

(c) $\mathfrak{L}_{\mathfrak{e}}$ *has a continuity property on cubes,*

then
(A) $\mathfrak{w} = t^{1+\sigma}$ *with* $\operatorname{sgn}\sigma \cdot \mathfrak{t}(N)$ *increasing,* $\sigma \in (-\infty, -1) \cup (0, \infty)$*;*
(B) for any $A \subset \Omega$ *compact, with* $C_{\mathfrak{e}} = \mathfrak{L}_{\mathfrak{e}}(\boldsymbol{q}_d)$*,*

$$\mathfrak{L}_{\mathfrak{e}}(A) = \frac{C_{\mathfrak{e}}}{(\lambda_d(A))^{\sigma}}$$

(C) optimizers $\omega_N^*(A)$ *converge to the uniform probability measure, for any compact* $A \subset \Omega$ *with* $\lambda_d(A) > 0$*.*

- σ is determined by the scaling properties of $\mathfrak{e}$.
- Curious: the rate is necessarily a power function, up to a slowly-varying factor:

$$\mathfrak{t}(N) = \varphi(N) \cdot N^{1+\sigma}$$

- Adding weight works too: if $\eta : \Omega \to [h_0, \infty]$, $h_0 > 0$,

$$Z(x + a\boldsymbol{q}_d; \eta) = \left\{ \eta(y) \cdot \frac{C_{\mathfrak{e}}}{[(a^d)]^\sigma} : y \in (x + a\boldsymbol{q}_d) \right\},$$

then

$$\min Z \leqslant \mathfrak{L}_{\mathfrak{e}}(x + a\boldsymbol{q}_d) \leqslant \max Z$$

implies

$$\mathfrak{L}_{\mathfrak{e}}(A) = \frac{C_{\mathfrak{e}}}{\left(\int_A \eta^{-1/\sigma} \mathrm{d}\lambda_d\right)^\sigma}$$

for all compact $A \subset \Omega$.

- For long-range interactions we had

$$\frac{1}{N^2} E_s(\omega_N^*) \to \iint_A \|x-y\|^{-s} \, d\mu(x)\mu(y), \qquad N \to \infty$$

- Extend $\mathfrak{e}$ from discrete configurations to all measures:

$$\mathfrak{e}_N(\mu, A) = \begin{cases} \mathfrak{e}(\omega_N, A), & \mu = \frac{1}{N}\sum_i \delta_{x_i}; \\ +\infty, & \text{otherwise,} \end{cases}$$

- Consider

$$\lim_{N\to\infty} \frac{\mathfrak{e}_N(\cdot, A)}{\mathfrak{t}(N)}$$

(limit of functionals)

Gamma-convergence

- The functional

$$\mu \mapsto C_{\mathfrak{e}} \int_A \eta(x)\, h(x)^{1+\sigma}\, d\lambda_d(x)$$

with

$$h = d\mu/d\lambda_d$$

is the continuous counterpart of the discrete problem now.

- It is the Gamma-limit of $\mathfrak{e}_N$, so in particular

$$\liminf_{N\to\infty} \frac{\mathfrak{e}_N(\mu_N, A)}{\mathfrak{t}(N)} \geqslant C_{\mathfrak{e}} \int_A \eta(x)\, h(x)^{1+\sigma}\, d\lambda_d(x)$$

when $\mu_N \rightharpoonup \mu$, and for some sequence $\{\mu_N^*\}$ the equality is achieved

A tale of two problems

- optimal quantizers
- Riesz interactions
- Persson-Strang meshing algorithm

A tale of three problems

Nobody expects the Spanish inquisition!

Figure: A result of Monty Python (1970)

Persson-Strang meshing algorithm

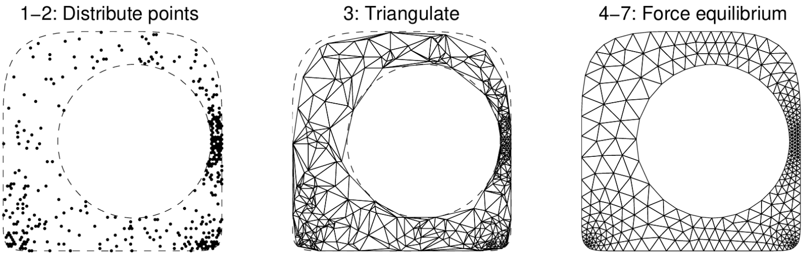


Figure: Persson-Strang (2004)

- Dynamics with the update

$$\omega_N^{n+1} = \omega_N^n + \Delta t F(\omega_N^n),$$

- where F is the sum of Delaunay edge forces, which depend on edge length l through

$$f(l, l_0) = 1.2(l_0 - l)_+,$$

- $$l_0 = \left(\frac{1}{N}\sum_i l_i^2\right)^{1/2}$$

Persson-Strang as a short-range functional

- Integral functional for the above dynamics is

$$\frac{1}{2}\mathfrak{e}(\omega_N) = \sum_{i=1}^{N} \sum_{j \in T_i} \left((1+P) \cdot \left(\frac{\sum_{i \geqslant 1, l \in T_i} \|x_l - x_i\|^2}{2 \sum_{i=1}^{N} \# T_i} \right) - \|x_j - x_i\|^2 \right)_+ ,$$

for a fixed $P > 0$ and the Delaunay edges connecting (x_i, x_j) with $j \in T_i$.

- Quadratic scaling means $\sigma = -2/d$, $-1 \leqslant \sigma < 0$, so the optimal configurations $\omega_N^*(A)$ now denote maximizers of $\mathfrak{e}(\omega_N)$.

- With the additional assumption that $T_i \subset I_{i,k}$ for some large k, we obtain asymptotic characterization for the maximizers.

Theorem (Hardin-Saff-V, 2020+)

Suppose $d \geqslant 3$ and $T_i \subset I_{i,k}$ for all i. Then the maximizers of Persson-Strang with weight η satisfy

$$\lim_{N\to\infty} \frac{\sup_{\omega_N \subset A} \mathfrak{e}(\omega_N)}{N^{1-2/d}} = C_{\mathfrak{e}} \left(\int_A \eta^{d/2}\, d\lambda_d \right)^{2/d}$$

with the optimal configurations converging to $\eta^{1-2/d}$, normalized.

Question

What are the asymptotics for $d = 2$?

Shimada-Gossard algorithm

- Shimada-Gossard (1998) proposed a meshing algorithm based on packing interacting bubbles.

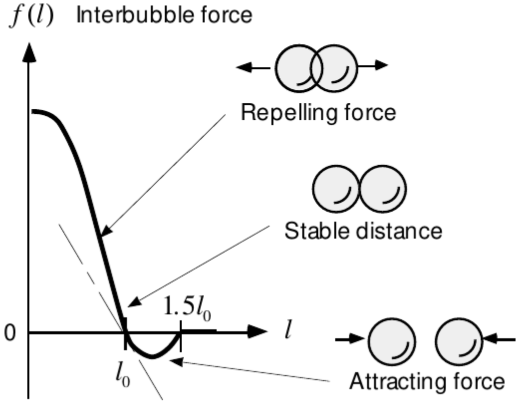


Figure: The graph of the "interbubble force".

- Andrade-Vyas-Shimada (2015) packs anisotropic bubbles!

Shimada-Gossard with nonuniform density

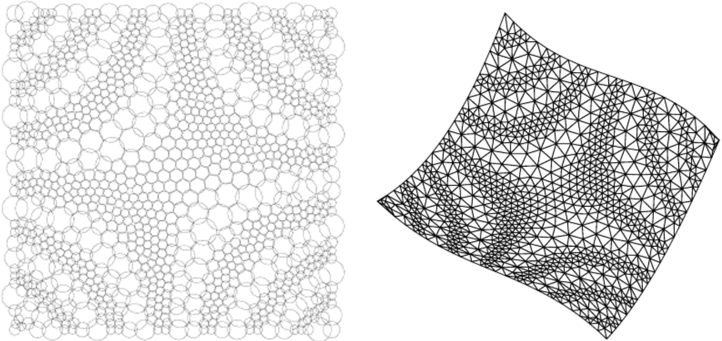


Figure: Packed bubbles and their Delaunay triangulation.

Some open problems

- What other short-range interactions are there? For example, in Petrache-Serfaty (2017), it is shown that the asymptotics of the second-order term for the Riesz energy, $d-2 \leqslant s < d$, is determined by

$$C_{s,d} \int h^{1+s/d}\, d\lambda_d(x)$$

with $h = d\mu^*/d\lambda_d$, the density of the minimizer of

$$\mu \mapsto \iint \|x-y\|^{-s}\, d\mu(x)d\mu(y) + \int V(x)\, d\mu(x)$$

- Is it possible to bound the degree of the Delaunay mesh in Persson-Strang?
- Can Shimada-Gossard be treated within the same framework?
- What about angles, degrees in Delaunay triangulations of Riesz minimizers?

Conjecture

Second-order term of the Riesz energy behaves as a short-range interaction.

Conjecture

Optimizers of the Shimada-Gossard interaction are uniformly distributed.

Thank you!

Graf, S., & Luschgy, H. (2000). Foundations of quantization for probability distributions. Berlin; New York: Springer.

Borodachov, S. V., Hardin, D. P., & Saff, E. B. (2019). Discrete energy on rectifiable sets. Springer.

Gruber, P. M. (2004). Optimum quantization and its applications. Advances in Mathematics, 186(2), 456–497. doi:10.1016/j.aim.2003.07.017