Optimal polarization and covering on sets of low smoothness

Alex Vlasiuk

Vanderbilt University

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Setup

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

- Goal: study the quantity

$$\rho^*(A, N) = \inf_{\omega_N \subset \mathbb{R}^p} \sup_{y \in A} \operatorname{dist}(y, \omega_N)$$

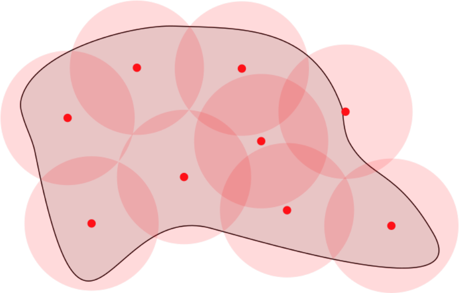
when $N \to \infty$. Also, study the limiting distribution of optimal ω_N.

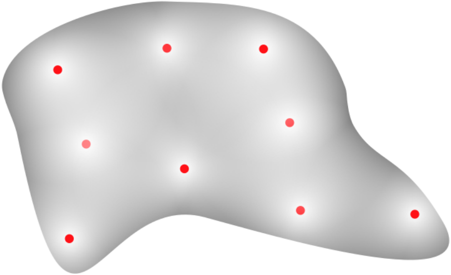
- Goal: study the quantity

$$\mathcal{P}_s^*(A, N) = \sup_{\omega_N \subset \mathbb{R}^p} \inf_{y \in A} \sum_{x \in \omega_N} \|y - x\|^{-s}.$$

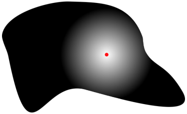
Symbol * denotes unconstrained optimization over ω_N.

Pictures





Left: covering with $N = 9$ points. Right: polarizing with $N = 9$ points, $s > 2$.
Below: a single point in a dark set, for comparison.



Some backstory: why $N \to \infty$?

- Metric entropy: Kolmogorov reads Shannon[1] and decides to extend entropy to geometry. He introduces ϵ-entropy of a compact set A as $\log_2 N_\epsilon(A)$, then considers

$$\lim_{\epsilon \downarrow 0} \frac{\log_2 N_\epsilon(A)}{\log_2(1/\epsilon)}$$

where $N_\epsilon(A) =$ smallest cardinality of an ϵ-covering of A

- Elements of ω_N encode A in the same sense as analog signals are encoded by the quantizer (Shannon's motivation)
- limit $N \to \infty$ determines complexity of set A

Kolmogorov-Tikhomirov study complexity of functional spaces. This became a big area subsequently (related to small ball inequality).

[1] as well as Hausdorff and Pontryagin-Shnirelman.

Some sidestory

- Shannon also considers a similar object: smallest transport distance from a measure supported on ω_N to a fixed continuous measure μ:

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

$\mathcal{F}_N$ – functions taking at most N values in $\mathbb{R}^d$

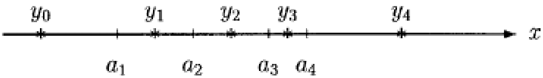


Figure: Quantization scheme with the quantizer $f(x) = \sum_i y_i 1_{S_i}(x)$

- Formally,

$$\inf_{\omega_N \subset \mathbb{R}^d} M_p(\omega_N; \mu_\xi) \qquad \text{with } M_p(\omega_N; \mu_\xi) = \int \min_{y_i \in \omega_N} \|x - y_i\|^p \, d\mu_\xi(x)$$

...and some frontstory

- Kolmogorov-Tikhomirov establish existence of the limit for Jordan-measurable sets; proof rediscovered 40 years later.

Theorem (Kolmogorov-Tikhomirov 1959; Graf-Luschgy 2000)

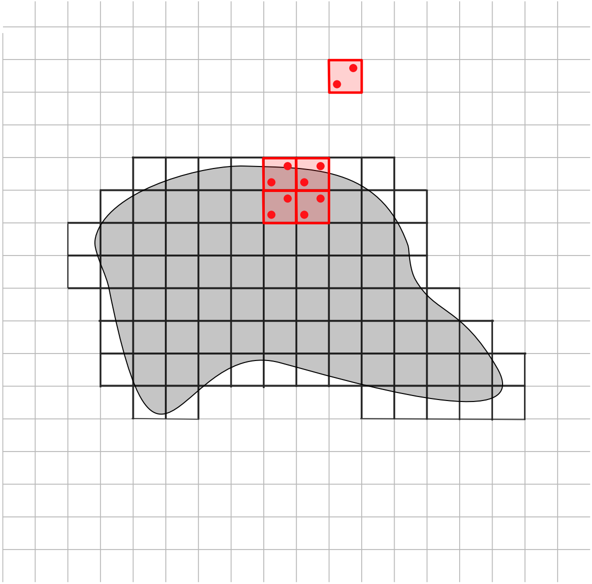
Given a nonempty compact $A \subset \mathbb{R}^d$ with $\mathcal{H}_d(\partial A) = 0$, one has

$$\lim_{N\to\infty} N^{1/d}\rho^*(A, N) = \theta_d \mathcal{H}_d(A)^{1/d},$$

with the finite positive constant θ_d depending only on the dimension d and the norm chosen in $\mathbb{R}^d$.

- Graf-Luschgy conjectured that the same holds when $\mathcal{H}_d(\partial A) > 0$.

Idea of the proof for Jordan-measurable sets



Meanwhile, polarization

Theorem (Borodachov-Hardin-Reznikov-Saff 2018; Hardin-Saff-Petrache 2020)

Given a nonempty compact $A \subset \mathbb{R}^d$ with $\mathcal{H}_d(\partial A) = 0$, one has for every $s > d$,

$$\lim_{N\to\infty} \frac{\mathcal{P}_s(A, N)}{N^{s/d}} = \lim_{N\to\infty} \frac{\mathcal{P}_s^*(A, N)}{N^{s/d}} = \frac{\sigma_{s,d}}{\mathcal{H}_d(A)^{s/d}},$$

where the finite positive constant $\sigma_{s,d}$ depends on s, d, and the used norm only.

- Why is $s > d$ necessary?
- Why the smoothness assumption?

Short-range interactions

By Hardin-Saff-V 2020: every sequence of functionals $\mathfrak{e}(\omega_N, A)$ acting on

$$\mathfrak{e} : (\mathbb{R}^d)^N \times \mathcal{C}(\mathbb{R}^d) \to [0, \infty]$$

has asymptotics and uniform distribution $N \to \infty$ on compact subsets of $\mathbb{R}^d$, provided it is

- monotonic in A:

$$\mathfrak{e}(\omega_N, A) \geqslant \mathfrak{e}(\omega_N, B) \qquad \text{for} \quad A \subset B$$

- has translation-invariant limits on cubes:

$$\lim_{N\to\infty} \frac{\mathfrak{e}(\omega_N^*,\ x + a[0,1]^d)}{N^\sigma} = f(a).$$

- short-range: for A_1, A_2 positive distance apart, $A = A_1 \cup A_2$

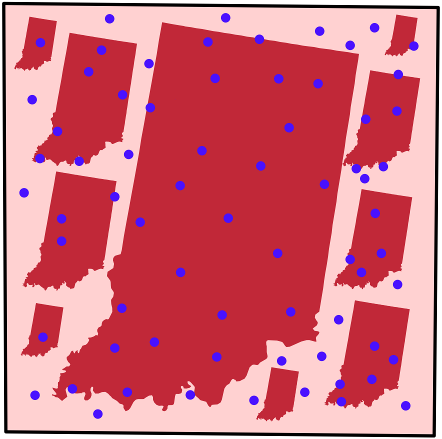
$$\lim_{N\to\infty} \frac{\mathfrak{e}(\omega_N \cap A_1, A_1) \star \mathfrak{e}(\omega_N \cap A_2, A_2)}{\mathfrak{e}(\omega_N, A)} = 1.$$

- $\mathfrak{e}$ is asymptotically stable under perturbations of ω_N and A

Stability allows to extend to non-smooth sets

- fraction of points used to cover small volumes is small, even if the shape of these small volumes is very rough
- If Indianas occupy at least $1-\delta(\epsilon)$ fraction of the volume,

$$\lim_{N\to\infty} \frac{\mathfrak{e}(\omega_N \cap [0,1]^2, [0,1]^2)}{N^\sigma} \geqslant (1-\epsilon) \limsup_{N\to\infty} \frac{\mathfrak{e}(\omega_N \cap \boldsymbol{IN}, \boldsymbol{IN})}{N^\sigma}$$



Covering functional is short-range!

Theorem (Anderson-Reznikov-V-White, 2022)

For any compact $(\mathcal{H}_d, d)$-rectifiable $A \subset \mathbb{R}^p$ satisfying $\mathcal{H}_d(A) = \mathcal{M}_d(A)$ one has

$$\lim_{N\to\infty} N^{1/d}\rho(A,N) = \lim_{N\to\infty} N^{1/d}\rho^*(A,N) = \theta_d \mathcal{H}_d(A)^{1/d},$$

with the constant θ_d depending only on the dimension d and the norm chosen in $\mathbb{R}^p$. In particular, the above holds for any compact set $A \subset \mathbb{R}^d$.

Polarization for $s > d$ is also short-range

Theorem (Anderson-Reznikov-V-White, 2022)

For any compact $(\mathcal{H}_d, d)$-rectifiable set $A \subset \mathbb{R}^p$ satisfying $\mathcal{H}_d(A) = \mathcal{M}_d(A)$ one has, for $s > d$,

$$\lim_{N\to\infty} \frac{\mathcal{P}_s(A,N)}{N^{s/d}} = \lim_{N\to\infty} \frac{\mathcal{P}_s^*(A,N)}{N^{s/d}} = \frac{\sigma_{s,d}}{\mathcal{H}_d(A)^{s/d}},$$

with the constant $\sigma_{s,d}$ depending only on the dimension d, exponent s, and the norm chosen in $\mathbb{R}^p$. In particular, the above holds for any compact set $A \subset \mathbb{R}^d$.

Theorem (Anderson-Reznikov-V-White, 2022)

Assume $A \subset \mathbb{R}^p$ is a compact $(\mathcal{H}_d, d)$-rectifiable set satisfying $\mathcal{H}_d(A) = \mathcal{M}_d(A) > 0$. Let $\{\omega_N\}_{N=1}^{\infty}$ be any sequence of configurations in $\mathbb{R}^p$ such that

$$\lim_{N\to\infty} N^{1/d} R(\omega_N, A) = \theta_d \mathcal{H}_d(A)^{1/d}, \quad \text{or} \quad \lim_{N\to\infty} \frac{P_s(A,\omega_N)}{N^{s/d}} = \frac{\sigma_{s,d}}{\mathcal{H}_d(A)^{s/d}}.$$

Then the sequence of corresponding empirical measures satisfies

$$\frac{1}{N}\sum_{x\in\omega_N} \delta_x \xrightarrow{*} \frac{\mathcal{H}_d(\cdot \cap A)}{\mathcal{H}_d(A)},$$

with the convergence understood in the weak* sense.

…and so are a few others!

- Math. phys. community studied thermodynamic limits for large systems in the 60s–70s Ruelle, Fisher
- Persson-Strang 2004 produce a simple mesh generator which works by optimizing local interactions
- Gruber 2004 establishes asymptotics for the Shannon's optimal quantization on Jordan-measurable sets and manifolds
- Hardin-Saff 2005 establish asymptotics of hypersingular Riesz energies on rectifiable manifolds
- Cohn-Salmon 2021 study asymptotics of packing bound functions ϑ' with a similar strategy
- Hardin-Saff-V 2022 study Riesz s-energies with k-nearest neighbor truncation, $0 < s < d$

Fractals

- A compact $A \subset \mathbb{R}^p$ is a *self-similar fractal* with similitudes $\{\psi_m\}_{m=1}^{M}$ and their contraction ratios $0 < r_m < 1$, $1 \leqslant m \leqslant M$, if

$$A = \bigsqcup_{m=1}^{M} \psi_m(A).$$

- Our fractals satisfy the open set condition: for an open $V \supset A$,

$$\bigsqcup_{m=1}^{M} \psi_m(V) \subset V.$$

Theorem (Anderson-Reznikov-V-White, 2021)

Let A be a fractal set with similitudes $\{\psi_m\}_{m=1}^M$ and contraction ratios $\{r_m\}_{m=1}^M$. Let $s > d = \dim_H(A)$. If the set

$$\{t_1 \log(r_1) + \cdots + t_M \log(r_M) : t_1, \ldots, t_M \in \mathbb{Z}\}$$

is dense in $\mathbb{R}$, then the limits

$$\lim_{N\to\infty} \frac{\mathcal{P}_s^*(A,N)}{N^{s/d}}, \qquad \lim_{N\to\infty} \frac{\mathcal{P}_s(A,N)}{N^{s/d}}$$

exist.

- The corresponding result for covering on fractals is obtained in Lalley 1988.
- The proof applies renewal theorem to the optimal polarization functional.

Theorem (Anderson-Reznikov-V-White, 2021)

Let A be a fractal set defined by similitudes $\{\psi_m\}_{m=1}^M$ with contraction ratios $\{r_m\}_{m=1}^M$. Let $d = \dim_H(A)$ and $s > d$. If the set

$$\{t_1 \log(r_1) + \cdots + t_M \log(r_M) : t_1, \ldots, t_M \in \mathbb{Z}\}$$

is not dense in $\mathbb{R}$, then for large values of s the limit

$$\lim_{N\to\infty} \frac{\mathcal{P}_s^*(A, N)}{N^{s/d}}$$

does not exist.

Extra: renewal theory and idea of the fractal result

Theorem (Feller 1966)

Let μ be a probability measure on $[0,\infty)$ and $Z(u)$ be a function defined on $[0,\infty)$. Assume that for some positive constants C, ϵ, and u sufficiently large there holds

$$\left| Z(u) - \int_0^u Z(u-x)\, d\mu(x) \right| \leqslant Ce^{-\epsilon u}.$$

Then $\lim_{u\to\infty} Z(u)$ exists.

- To have a continuous argument, invert the functional: $N(t) := \min\{N \colon \mathcal{P}_s^*(A,N) \geqslant t\}$
- Derive $N(t) = L(t) + \sum_{m=1}^M N(tr_m^s)$ with $|L(t)| \leqslant Ct^{d/s-\epsilon}$

Conclusions

- Short-range interactions are nicer than long-range in that the asymptotics/distribution more often can be computed explicitly.
- Typical algorithms for generating a given distribution are short-range.
- Some typical interactions in physics and chemistry are short-range: hard core, Lennard-Jones potential, magnetic dipoles interactions, multipole interactions, etc.
- Still, short-range interactions without scale invariance can be hard to understand, with the limit depending on scaling – see the Lennard-Jones potential

$$\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}$$

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Thank you!

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