Log-energy, β -ensembles, and tessellations: problems old and new

Abstract

A collection of open problems discussed at the ICERM Optimal and Random Point Configurations workshop, held on February 26–March 2, 2018.

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1 Discrete log-energy

[Suggested by Carlos Beltrán.] Consider the logarithmic energy of an N-point subset of the two-dimensional sphere $x_1, \ldots, x_N \subset \mathbb{S}^2$, defined by

$$E_{\log}(oldsymbol{x}_1,\ldots,oldsymbol{x}_N) = \sum_{i
eq j} \log rac{1}{|oldsymbol{x}_i - oldsymbol{x}_j|}.$$

Its minimizers are known as the Fekete points and are related to the condition numbers of polynomials; additional motivation for considering this functional can be found in [30]. The common goal of the following questions is to characterize behavior of $E_{\log}: (\mathbb{S}^2)^N \to \mathbb{R}$ and the set on which the value of $\mathcal{E}_{\log}(N) := \min \{ E_{\log}(x_1, \dots, x_N) : x_i \in \mathbb{S}^2, 1 \leq i \leq N \}$ is attained.

1. How many critical points does E_{\log} have? How many are there under a certain level? What are they? It has been conjectured [16] that the number of critical points of $E_{\log}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N)$ is exponential in N. A result to this effect is known for probabilistic spin glass model [3, 31], where it follows via an application of Kac-Rice formula to the Hessian of a random matrix. Some numerical evidence for the harmonic kernel can be found in [14].

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2. Can one estimate values of E_{log} at the local and global minima, so that in some sense

$$E_{\log}(\text{local minimum}) \approx E_{\log}(\text{global minimum})$$
?

Empirical data seem to indicate that E_{log} has multiple different local minima values close to the global one [28, 16].

3. Let further x_1, \ldots, x_N be a Nash equilibrium of E_{\log} on \mathbb{S}^2 , that is,

$$E_{\log}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_i,\ldots,\boldsymbol{x}_N) = \min\left\{E_{\log}(\boldsymbol{x}_1,\ldots,\boldsymbol{x},\ldots,\boldsymbol{x}_N): \boldsymbol{x} \in \mathbb{S}^2\right\}, \quad 1 \leq i \leq N.$$

As shown in [5], under the additional assumption that $\operatorname{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) \geq 4 \arcsin \sqrt{\frac{\delta}{N}}$ for some $\delta \in (0, 1)$, there holds

$$E_{\log}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_i,\ldots,\boldsymbol{x}_N) \leq \left(\frac{1}{2} - \log 2\right) N^2 - \frac{\delta N \log N}{2}.$$

The natural question is: how can this be improved? The RHS here should be compared with the expansion from [7],

$$\mathcal{E}_{\log}(N) = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{N \log N}{2} + CN + o(N).$$

2 Equilibrium measures and Jacobi matrices of Cantor sets

[Suggested by Giorgio Mantica.] Let $E_n \subset \mathbb{R}$, $n \geq 1$ be a sequence of closed subsets of the real line such that $E_{n+1} \subset E_n$, and

$$E_n = \bigcup_{i=1}^{M^n} \left[\alpha_i^{(n)}, \, \beta_i^{(n)} \right],$$
$$E := \bigcap_{n \ge 1} E_n.$$

Here the union in the RHS is disjoint: $\alpha_{i+1}^{(n)} > \beta_i^{(n)}$. Assuming that the ratios $(\beta_j^{(n+1)} - \alpha_j^{(n+1)})/(\beta_i^{(n)} - \alpha_i^{(n)})$ are bounded uniformly in i, j, n, one arrives at a generalization of the classical Cantor set. Minimization of the continuous functional

$$I_{\log}(\mu) := \iint \log \frac{1}{|x - y|^p} d\mu(x) d\mu(y).$$

over probability measures supported on E_n defines an equilibrium measure ν_n ; there exists a corresponding sequence of orthogonal polynomials satisfying a three-term recurrence relation that can be written as a Jacobi matrix, which is well-known to be almost periodic [29, 27]. It is then natural to consider the classes of Jacobi matrices of measures on E_n and on E, and try to show that the latter is the limit of the former; in particular, establish almost-periodicity of Jacobi matrices arising from measures on E. This conjecture was initially formulated in [26], then revived and corroborated by numerical evidence in [23] and [27]; the reader can consult [27] for further references. At the time of writing, the numerical argument in [27] remains to be made rigorous.

Before giving the precise formulations, we recall the construction of the equilibrium measure of a collection of N intervals; in our context of generalized Cantor sets, $N = M^n$. Let

$$Y(z) = \prod_{i=1}^{N} (z - \alpha_i)(z - \beta_i),$$

and the gap polynomial

$$Z(z; \zeta_i) = \prod_{i=1}^{N-1} (z - \zeta_i),$$

where $\zeta_i \in (\beta_i, \alpha_{i+1})$, that is, inside the gaps of the support. Then, after choosing ζ_i 's so that

$$\int_{\beta_i}^{\alpha_{i+1}} \frac{Z(s)}{\sqrt{|Y(s)|}} ds = 0, \quad i = 1, \dots N - 1,$$

the density of the equilibrium measure of E_n can be written as

$$d\nu_n(s) = \frac{1}{\pi} \sum_{i=1}^N \mathbb{1}_{[\alpha_i, \beta_i]}(s) \frac{|Z(s)|}{\sqrt{|Y(s)|}} ds.$$

This sequence of measures has a weak* limit; it coincides with the equilibrium measure of E [27], and we shall denote it by ν_E .

1. Denote as before the equilibrium measure of the *n*-th set E_n by ν_n . Quantify the speed of the weak* convergence of ν_n ; in particular, is it true that for some $0 < \delta < 1$, the Wasserstein distance is bounded as

$$d_W(\nu_n, \nu_E) \le c \, \delta^n$$
?

2. The *isospectral torus* of a finite set of intervals is the collection of Jacobi matrices arising from the measures of the form

(Iso)
$$d\theta(s;\zeta_i) = \frac{A}{\pi} \sum_{i=1}^{N} \mathbb{1}_{[\alpha_i,\beta_i]}(s) \frac{\sqrt{|Y(s)|}}{|Z(s;\zeta_i)|} ds + \sum_{i=1}^{N} B_i \delta_{\zeta_i}.$$

where A, B_i are positive weights and θ is a positive measure, such that its Stieltjes transform

$$M(z) := \int \frac{d\theta(s)}{z - s},$$

can be written as

$$M(z) = \frac{X(z) - \sqrt{Y(z)}}{Z(z; \zeta_i)}$$

with X(z) a polynomial interpolating $\sqrt{Y(z)}$ at ζ_i 's. It is therefore natural to define the isospectral torus of the "infinite-gap" set E as the weak* limit of the finite measures θ as in (**Iso**); the obvious question is, does

$$\nu(\cdot;\zeta_i) \longrightarrow \nu_{\infty}(\cdot;\zeta_i)$$
?

If so, is the Jacobi matrix $J_{\nu_{\infty}}(\zeta_i)$ determined by

$$J_{\nu_{\infty}}(\zeta_i) \longrightarrow J_{\nu_{\infty}}(\zeta_i)$$

almost periodic?

3 β -ensembles

[Suggested by Paul Bourgade.] Recall that the density of a β -ensemble is defined by

(
$$m{eta}$$
) $\mu^{(N)}(dm{z}) = \frac{1}{Z_N^{\beta}} \prod_{i < j} |z_i - z_j|^{\beta} \prod_{i=1}^N e^{-N\beta V(z_i)} dz_1 \dots dz_N,$

where $z_i \in \mathbb{C}$, and V grows in a suitable way. This family of laws describes a number of important matrix models [2]; in addition, when the z_i 's are real, for a whole range of connections to Jacobi matrices from the previous section, consult one of [12, 22, 21].

1. When $\beta = 2$ and $V(z) = |z|^2$, (β) is the density of Ginibre ensemble; it is known (see e.g. [11] for this easy calculation) in this case that the pairwise correlation function decays exponentially in the bulk:

$$\rho_2^{(N)}(x,y) = 1 - e^{-N|x-y|^2} (1 + o(1)),$$

for any $0 < |x-y| \ll 1$. Is this still the case for a general V? This is proved when $|x-y| \approx N^{-1/2}$ is on the microsopic scale [1, Theorem 4.2], but unclear on mesoscopic scales. Moreover, for Ginibre ensemble, the correlation on the boundary decays polynomially [13]; does this apply to a more general case?

2. Consider the Ginibre ensemble again; let $\Omega \in D$, where D is the unit disk in \mathbb{C} , and let $\operatorname{len}[\partial\Omega] < \infty$; that is, $\partial\Omega$ is rectifiable. Then there holds

(Fluct)
$$\operatorname{Var}(\#\{z_i \in \Omega\}) \simeq N^{1/2} \operatorname{len}[\partial \Omega], \quad N \to \infty.$$

What is the corresponding result for fractal domains satisfying $\text{len}[\partial\Omega] = \infty$? What is the quantity defining the exponent of N in (**Fluct**): Hausdorff dimension of Ω , its Minkowski content, etc.?

3. For a general value of β in the distribution (β), it is known [24, 4] that, for a smooth f,

$$\operatorname{Var}\left(\sum_{i=1}^{N}f(z_{i})\right) \approx 1, \quad N \to \infty.$$

There is, however, no "soft" argument justifying this; see for example [25, 15] for concentration in very general settings, but not up to the optimal fluctuation scale in the above example.

4. Assume that $V(z) = |z|^2$. What are the observables for which one could explicitly compute the expectation with respect to (β) ? One candidate, for example, is

$$\mathcal{C}(\gamma, N) = \mathbb{E}\left(\prod_{i=1}^{N} |z_i|^{\gamma}\right)$$

for a suitable power γ .

4 Tessellations and packings

[Suggested by Dmitriy Bilyk.] Denote the normalized spherical measure on \mathbb{S}^d by σ_d .

1. A question asked by L. Fejes Tóth concerns the areas of components of a tessellation of \mathbb{S}^d with arbitrary planes. Let S_1, S_2, \ldots, S_M be the cells obtained by the tessellation of \mathbb{S}^d with N hyperplanes. Then

$$\frac{\max \sigma_d(S_i)}{\min \sigma_d(S_i)} \to \infty,$$

as $N \to \infty$. The proof is not known even if one considers tessellations with random hyperplanes. Another motivation for this question comes from 1-bit compressed sensing [9].

[Suggested by Kenneth Stephenson.] On a related note, consider a bi-infinite cylinder $C := \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 : x_1^2 + x_2^2 \le 1\}$ in \mathbb{R}^3 . Our goal will be to fill the space between C and 2C with hard balls in the densest possible way; here of course 2C denotes a bi-infinite cylinder of radius 2 with the same axis. Specifically, let $B_i := B(x_i, 1/2), 1 \le i \le N$ be a collection of unit balls of diameter 1, centered in x_i 's, and define the density of this collection as

$$\Delta := \limsup_{H \to \infty} \frac{\sum_{i=1}^{N} \operatorname{vol} \left[B_i \cap ((2C)_H \setminus C_H) \right]}{\operatorname{vol} \left[2C_H \setminus C_H \right]},$$

where we write vol[·] for the Lebesgue measure in \mathbb{R}^3 and $A_H := \{ \boldsymbol{x} \in A : |x_3| \leq H \}$ is the truncation of a set $A \subset \mathbb{R}^3$ by planes $z = \pm H$. Packing of hard balls in a tube is a natural model of certain nanostructures, the fact that serves as a motivation for the following problems. Numerical simulations of this model using linear programming can be found for example in [19, 20]. Packing of balls confined by parallel planes has been discussed in [18].

- 1. What is the maximal value of Δ over all (infinite) collections of $\{x_i\}$, assuming that B_i touch C?
- **2.** Consider also natural modifications of this question, for example when the inner and outer cylinders are rC and (1+r)C with $r\gg 1$, etc. Do the projections of $\boldsymbol{x}_i,\ 1\leq i\leq N$, onto the boundary ∂C form hexagonal / periodic patterns for different r?

5 Orthogonalizing energies

[Suggested by Dmitriy Bilyk.] In this section,

$$I_f(\mu) := \iint\limits_{\mathbb{S}^d} f(\boldsymbol{x} \cdot \boldsymbol{y}) d\mu(\boldsymbol{x}) d\mu(\boldsymbol{y})$$

1. For vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^d$, define

$$\theta(\boldsymbol{x}, \boldsymbol{y}) = \min \left\{ \arccos(\boldsymbol{x} \cdot \boldsymbol{y}), \pi - \arccos(\boldsymbol{x} \cdot \boldsymbol{y}) \right\} = \arccos|\boldsymbol{x} \cdot \boldsymbol{y}|,$$

i.e. the acute angle between the lines containing $x, y \in \mathbb{S}^d$. Consider the discrete energy

$$E_{\theta}(\boldsymbol{x}_{1},...,\boldsymbol{x}_{N}) := \frac{1}{N^{2}} \sum_{i,j=1}^{N} \theta(\boldsymbol{x}_{i},\boldsymbol{x}_{j})$$

when the set $\{\boldsymbol{x}_1,...,\boldsymbol{x}_N\}\subset\mathbb{S}^d.$ Prove that

$$\max \left\{ E_{\theta}(\boldsymbol{x}_1,...,\boldsymbol{x}_N) \, : \, \{\boldsymbol{x}_1,...,\boldsymbol{x}_N\} \subset \mathbb{S}^d \right\} = E_{\theta}(\boldsymbol{e}_{i \bmod (d+1)}),$$

where e_j denotes the j-th orthonormal basis vector. In other words, a repeated orthogonal basis is a maximizer of this energy. This question and the conjecture are also due to Fejes Tóth.

2. Let $F(t) := \arccos|t|$; then the energy from the previous question can be extended to Borel measures supported on \mathbb{S}^d . Conjecture:

$$\max\left\{I_F(\mu): \mu \in \mathcal{P}_1(\mathbb{S}^d)\right\} = I_F\left(\frac{1}{N} \sum_{i=1}^N \delta_{\boldsymbol{e}_{i \bmod (d+1)}}\right) = \frac{\pi}{2} \cdot \frac{N-1}{N},$$

where the minimum is taken over probability measures supported on \mathbb{S}^d , and the notation for basis elements is again e_j . The conjecture has been proved for d=1. For partial progress including an asymptotic bound see [17]; for an improved bound obtained with different methods consult also [10].

3. Let $f(t) = |t|^p$ with p > 0. Consider, as above, the discrete and continuous energy with the following kernel:

$$E_{f_p}(\boldsymbol{x}_1,...,\boldsymbol{x}_N) = \frac{1}{N^2} \sum_{i,j=1}^N |\boldsymbol{x}_i \cdot \boldsymbol{x}_j|^p \quad \text{ and } \quad I_{f_p}(\mu) = \iint_{\mathbb{S}^d} |\boldsymbol{x} \cdot \boldsymbol{y}|^p d\mu(\boldsymbol{x}) d\mu(\boldsymbol{y}).$$

In view of the previous question, the motivation for minimizing an energy with kernel f_p is that it arises in the asymptotic expansion of $\operatorname{arccos} | \boldsymbol{x} \cdot \boldsymbol{y}|$. It turns out, potential with the f_2 kernel is well-known as the "frame potential", and the minimizers of E_{f_2} can be characterized as tight frames [6]. Examples of TFs in any dimension are the (regular) simplex and orthonormal bases. Furthermore, the continuous functional I_{f_2} for p=2 is minimized on every measure with the second moment proportional to the identity matrix: $\mathbb{E}_{\boldsymbol{x} \sim \mu} \boldsymbol{x} \boldsymbol{x}^T = c \mathbb{1}_{d+1}$. For $0 , ONB is a minimizer of <math>I_{f_p}$, and the spherical measure σ_d isn't; for any even p > 2, σ_d is a minimizer (the ONB is not). It has been established recently [8] that an antipodal spherical design of degree 2m-1 that has at most m scalar products, minimizes E_{f_p} ; the same applies to a non-antipodal design of degree 2m.

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