

Mathematical Institute

Global minimizers of Interaction Energies

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Collective behavior

macroscopic individuals: animals





microscopic individuals: bacteria





First-order models with attractiverepulsive pairwise interactions

$$\dot{\mathbf{x}}_i = -\frac{1}{N} \sum_{j=1,\dots,N, \ j \neq i} \nabla W(\mathbf{x}_i - \mathbf{x}_j) \qquad i = 1,\dots,N$$

• $\mathbf{x}_i(t)$: location of the i-th individual

- $W = W(r), r = |\mathbf{x}|$ radial interaction potential
- Usually used for micro-organisms, where inertia can be neglected.



Energy structure

$$\dot{\mathbf{x}}_i = -\frac{1}{N} \sum_{j=1,\dots,N, \ j \neq i} \nabla W(\mathbf{x}_i - \mathbf{x}_j) \qquad i = 1,\dots,N$$

It is the gradient flow of the energy functional

$$E(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \frac{1}{2N^2} \sum_{i,j:i\neq j} W(\mathbf{x}_i - \mathbf{x}_j)$$

- Energy dissipation rate $\frac{dE}{dt} = -\frac{1}{N}\sum_{i} |\dot{\mathbf{x}}_{i}|^{2}$
- Expected large time behavior: convergence to local energy minimizers

Question: Existence/Uniqueness of global/local energy minimizers?

How do they look like?



Energy minimizers

- Large time simulation: Kolokolnikov-Sun-Uminsky-Bertozzi
 11'

 -W'(r) = F(r) = tanh [(1 r)a] + b; 0 < a; -tanh(a) < b < 1.
- Very complicated
- Break of symmetry





Continuum formulation

• Particle density function $\rho(t, \mathbf{x})$

• Energy
$$E = \frac{1}{2} \int \int W(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) d\mathbf{y} \rho(\mathbf{x}) d\mathbf{x}$$

Wasserstein-2 gradient flow

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \ \mathbf{u}(t, \mathbf{x}) = -\int \nabla W(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) d\mathbf{y}$$

 $\mathbf{u}(t, \mathbf{x})$: transport velocity

Energy dissipation rate

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\int |\mathbf{u}|^2 \rho \mathrm{d}\mathbf{x}$$

"Characterization" of Energy minimizers

- Steady states: $\nabla V = 0$ on $\operatorname{supp}\rho$, or $V = W * \rho$ is constant on each connected component of $\operatorname{supp}\rho$
- (Wasserstein-∞) local minimizers: further, V is larger nearby
- Global minimizers



 $V = W * \rho$: potential generated by ρ

Dimensionality of minimizers

Balagué-C.-Laurent-Raoul 13': if

$$\Delta W(x) \sim -\frac{1}{|x|^{\beta}} \text{ as } x \to 0 \qquad 0 < \beta < d$$

then the Hausdorff dimension of any Wasserstein- ∞ local minimizer is $\geq \beta$



Part 1: Linear interpolation convexity: uniqueness of local minimizers

E as a quadratic form

$$E[\rho] = \frac{1}{2} \int \int W(\mathbf{x} - \mathbf{y})\rho(\mathbf{y}) d\mathbf{y}\rho(\mathbf{x}) d\mathbf{x}$$

Define an associated bilinear form

$$\begin{split} E[\rho_1, \rho_2] &= \int \int W(\mathbf{x} - \mathbf{y}) \rho_2(\mathbf{y}) \mathrm{d}\mathbf{y} \rho_1(\mathbf{x}) \mathrm{d}\mathbf{x} \\ &= \int (W * \rho_2)(\mathbf{x}) \rho_1(\mathbf{x}) \mathrm{d}\mathbf{x} \quad \rho_1 \text{ in the potential generated by } \rho_2 \\ &= \int (W * \rho_1)(\mathbf{x}) \rho_2(\mathbf{x}) \mathrm{d}\mathbf{x} \quad \rho_2 \text{ in the potential generated by } \rho_1 \end{split}$$

Linear interpolation convexity (LIC)

• **Definition**: W has LIC property if for given ρ_0 and ρ_1 with the same total mass and center of mass, the function:

 $t \mapsto E[(1-t)\rho_0 + t\rho_1]$

is strictly convex on $0 \le t \le 1$

- LIC is basically the positive-definiteness of E as a quadratic form. $\frac{d^2}{dt^2}E[(1-t)\rho_0 + t\rho_1] = 2E[\rho_1 - \rho_0]$
- LIC potentials have unique global minimizer (for fixed total mass and center of mass). E



Linear interpolation convexity (LIC)

• LIC property can be guaranteed by Fourier transform:

$$E = \frac{1}{2} \int \int W(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) d\mathbf{y} \rho(\mathbf{x}) d\mathbf{x} = \frac{1}{2} \int \frac{\hat{W}(\xi) |\hat{\rho}(\xi)|^2 d\xi}{\text{form in } \rho}$$

Eigenvalues $\hat{W}(\xi) > 0$

Lopes 19' uses this to prove the LIC property of power-law potentials

$$W(\mathbf{x}) = \frac{|\mathbf{x}|^a}{a} - \frac{|\mathbf{x}|^b}{b} \qquad 2 \le a \le 4, \ -d < b < 0$$

and therefore obtain uniqueness and radial symmetry of global minimizers. Similar use for uniqueness by Frank 21', Davies-Lim-McCann 21'.

- Equivalent to: $E[\mu] > 0$ for any signed measure μ with $\int \mu = \int \mathbf{x}\mu = 0$
- Almost equivalent to $\hat{W}(\xi) \ge 0, \quad \forall \xi$

LIC applied to local minimizers: radial symmetry

- Theorem (C.-Shu 21'): in 2D, assume W has LIC property. Then compactly supported local minimizers *ρ* are radiallysymmetric.
- **Proof**: suppose ρ is a local minimizer which is not radially-symmetric.

• (1) By LIC,
$$\rho_{\theta} := \frac{1}{2}(\rho + \mathcal{R}_{\theta}\rho)$$
 has lower energy than ρ .
 \mathcal{R}_{θ} : rotate by θ around its center of mass 0

• (2) ρ_{θ} has higher energy than ρ by minimizing property, since ρ_{θ} is close to ρ in Wasserstein- ∞ . Contradiction!

Part 2: Linear interpolation concavity: small scales and fractals

Dimensionality of minimizers

Balagué-C.-Laurent-Raoul 13': if

$$\Delta W(x) \sim -\frac{1}{|x|^{\beta}}$$
 as $x \to 0$ $0 < \beta < d$

then the Hausdorff dimension of any local minimizer is $\geq \beta$

- β needs not to be an integer, but it was never observed that a local minimizer has non-integer dimension.
- We will show that non-integer dimension is possible.

Concavity

• **Definition**: *W* is infinitesimal-concave if for any $\delta > 0$ there exists $\mu \in L^{\infty}$ with $\int \mu d\mathbf{x} = 0$ and $\operatorname{diam}(\operatorname{supp} \mu) \leq \delta$ such that $E[\mu] < 0$

recall that LIC basically says $E[\mu] > 0$

 Lemma (C.-Shu 21'): if W is infinitesimal-concave, then for any local minimizer ρ, "suppρ" does not contain any interior point.

Concavity



Concavity by Fourier transform

- Recall that LIC corresponds to $\hat{W}(\xi) > 0$, $\forall \xi \neq 0$
- Lemma (C.-Shu 21'): Suppose W has certain regularity+growth, and for any R > 0, there exists such that $J \subset \mathbb{R}_+$, |J| = R

$$\hat{W}(\xi) < -c_1 R^{-\alpha}, \forall |\xi| \in J$$

Then W is infinitesimal-concave.













Part 3: Anisotropic Potentials

Dislocations in crystals



Edge dislocation

Screw dislocation

Pictures from https://www.doitpoms.ac.uk/tlplib/dislocations

Dislocations in crystals

- Phenomenological dislocation models have been derived in literature
- Each dislocation can be viewed as a particle
- Number of dislocations can be huge (say, $10^{15} m^{-2}$)
- It is typical to use a continuum model to describe the spatial configuration of dislocations, i.e., use a density function
- Roy-Peerlings-Geers-Kasyanyuk 08', Geers-Peerlings-Peletier-Scardia 13'

Minimization of 2D interaction energy

$$E[\rho] = \frac{1}{2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} W(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) \, \mathrm{d}\mathbf{y} \rho(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

- ho : density of dislocations, a probability measure on \mathbb{R}^2
- W : anisotropic interaction potential;
- Ω describes the anisotropy $W(\mathbf{x}) = |\mathbf{x}|^{-s} \Omega(\theta) + |\mathbf{x}|^2, \quad 0 < s < 2$ $\frac{\mathbf{x}}{|\mathbf{x}|} = (\cos \theta, \sin \theta)$ anisotropic repulsion attraction/confinement
- Logarithmic (s=0) case: $W_{\log}(\mathbf{x}) = -\ln |\mathbf{x}| + \Omega(\theta) + |\mathbf{x}|^2$



Previous results

- Similar ellipse-shaped minimizers are obtained in 3D in C.-Mateu-Mora-Rondi-Scardia-Verdera 21'
- Ellipse-shaped minimizers are obtained in 2D for a perturbed logarithmic potential in Mateu-Mora-Rondi-Scardia-Verdera 21'
- Questions: General singularity? General ω ? Ellipses / Collapse to lower-dimensions?



LIC and Euler-Lagrange condition

$$E[\rho] = \frac{1}{2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} W(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) \, \mathrm{d}\mathbf{y} \rho(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

Euler-Lagrange condition for energy minimizers (Balagué-Carrillo-Laurent-Raoul 13'):

 $(W * \rho)(\mathbf{x}) \leq \operatorname{essinf}(W * \rho), \quad \rho \ a.e.$

($W * \rho$ achieves min on $\operatorname{supp} \rho$)

- Theorem (CMMSRV 20', C.-Shu 21'): for LIC potentials, the unique energy minimizer is the only probability measure satisfying the E-L condition (up to translation).
- The ellipse-shaped minimizers in CMMSRV 20' are proved by verifying E-L condition explicitly

Fourier transform of anisotropic potential

- Assume Ω is smooth and $\Omega(\theta + \pi) = \Omega(\theta)$
- Lemma (C.-Shu 22'):

$$\mathcal{F}[|\mathbf{x}|^{-s}\Omega(\theta)] = |\xi|^{-2+s}\tilde{\Omega}(\varphi), \quad 0 < s < 2$$

$$\tilde{\Omega}(\varphi) = \tau_{2-s} \int_{-\pi}^{\pi} |\cos(\varphi - \theta)|^{-2+s} \Omega(\theta) \,\mathrm{d}\theta, \quad 1 < s < 2.$$

Applying reversely, we get

$$\Omega(\theta) = \tau_s \int_{-\pi}^{\pi} |\cos(\theta - \varphi)|^{-s} \tilde{\Omega}(\varphi) \, \mathrm{d}\varphi, \quad 0 < s < 1.$$

LIC for anisotropic energy

 $W(\mathbf{x}) = |\mathbf{x}|^{-s} \Omega(\theta) + |\mathbf{x}|^2, \quad 0 < s < 2$

• Theorem (C.-Shu 22'): W has the LIC property if and only if $\mathcal{F}[|\mathbf{x}|^{-s}\Omega(\theta)] = |\xi|^{-2+s}\tilde{\Omega}(\varphi)$ with $\tilde{\Omega} \ge 0$

$$|\mathbf{x}|^{-s}\Omega(\theta) = \tau_s \int_{-\pi}^{\pi} |\mathbf{x} \cdot \vec{e}_{\varphi}|^{-s} \tilde{\Omega}(\varphi) \,\mathrm{d}\varphi$$

- Notice that LIC is strict convexity but the Fourier condition is non-strict inequality. This comes from a complex analysis argument.
- If LIC fails, then W is infinitesimally concave (C.-Shu 21'), implying superlevel sets of any Wasserstein-infinity local minimizer do not contain interior points. This strongly suggests that minimizers collapse to lower dimensions.

LIC for anisotropic energy

 $W_{\alpha}(\mathbf{x}) = |\mathbf{x}|^{-s} (1 + \alpha \omega(\theta)) + |\mathbf{x}|^2 \qquad \hat{W}_{\alpha}(\xi) = |\xi|^{-2+s} (c_s + \alpha \tilde{\omega}(\theta))$

• If 0 < s < 1, then there exists a threshold



• If $1 \le s < 2$, then LIC always holds.

Part 3.1: Ellipse-shaped minimizers for the LIC case

Ellipse-shaped minimizers

• For 0 < s < 2, the minimizer for the isotropic potential $|\mathbf{x}|^{-s} + |\mathbf{x}|^2$ is $\rho_2(\mathbf{x}) = C_2(R_2^2 - |\mathbf{x}|^2)_+^{s/2}$

(Caffarelli-Vázquez 11', C.-Huang 17', C.-Shu 21')

• Rescaled and rotated version:

$$\rho_{a,b}(\mathbf{x}) = \frac{1}{ab} \rho_2 \left(\frac{x_1}{a}, \frac{x_2}{b} \right), \quad \rho_{a,b,\eta}(\mathbf{x}) = \rho_{a,b}(\mathcal{R}_{-\eta}\mathbf{x})$$

 These densities are supported on possibly degenerate ellipses



 bR_2

Ellipse-shaped minimizers

- Theorem (C.-Shu 22'): For 0 < s < 1, $W(\mathbf{x}) = |\mathbf{x}|^{-s} \Omega(\theta) + |\mathbf{x}|^2$
 - If $\tilde{\Omega} \ge c > 0$, then the unique energy minimizer is $\rho_{a,b,\eta}$ some a, b > 0 with $(a,b) \in [0,\infty)^2 \setminus \{(0,0)\}$
 - If $\tilde{\Omega} \ge 0$, then it is some $\rho_{a,b,\eta}$ with a=0 possibly.
- This result covers all LIC cases

 $\begin{array}{c|c} & & & \\ 0 & & \\ \text{LIC, ellipses} & & \\$

Key lemma

- By LIC, it suffices to verify the Euler-Lagrange condition, i.e., carefully calculate the potential generated by $\rho_{a,b,\eta}$
- Lemma (C.-Shu 22'): For 0 < s < 1,

 $(|\mathbf{x}|^{-s}\Omega(\theta) + Ax_1^2 + Bx_2^2 + 2Dx_1x_2) * \rho_{a,b} = C_{\Omega,a,b}, \quad \mathbf{x} \in \operatorname{supp} \rho_{a,b}$

$$\begin{pmatrix} A(a,b) \\ B(a,b) \\ D(a,b) \end{pmatrix} = \tau_s (R_1/R_2)^{2+s} \int_{-\pi}^{\pi} (a^2 \cos^2 \varphi + b^2 \sin^2 \varphi)^{-(2+s)/2} \begin{pmatrix} \cos^2 \varphi \\ \sin^2 \varphi \\ \cos \varphi \sin \varphi \end{pmatrix} \underline{\tilde{\Omega}(\varphi)} \, \mathrm{d}\varphi$$

If $\ \Tilde{\Omega} \geq 0$, then the generated potential is larger outside support

• This implies theorem by finding correct a, b, η to make

$$A = B = 1, D = 0$$

Sketch of proof

 $\mathcal{F}[|\mathbf{x}|^{-s}\Omega(\theta)] = |\xi|^{-2+s}\tilde{\Omega}(\varphi) \qquad \Omega(\theta) = \tau_s \int_{-\pi}^{\pi} |\cos(\theta - \varphi)|^{-s}\tilde{\Omega}(\varphi) \,\mathrm{d}\varphi, \quad 0 < s < 1.$

Decomposition of anisotropic potential into 1D potentials

$$|\mathbf{x}|^{-s} \Omega(\theta) = \tau_s \int_{-\pi}^{\pi} |\mathbf{x} \cdot \vec{e}_{\varphi}|^{-s} \tilde{\Omega}(\varphi) \, \mathrm{d}\varphi.$$

1D potential along φ

- To calculate $|\mathbf{x}|^{-s}\Omega(\theta) * \rho_{a,b}$, we calculate $|\mathbf{x} \cdot \vec{e_{\varphi}}|^{-s} * \rho_{a,b}$ and assembly
- The push-forward of $\rho_{a,b}$ by the projection operator onto $\vec{e_{\varphi}}$ is a rescaling of the 1D energy minimizer for the potential

$$|x|^{-s} + |x|^2$$



Sketch of proof

$$\left(\left(|\mathbf{x}\cdot\vec{e}_{\varphi}|^{-s} + \left(\frac{R_{1}}{r_{\varphi}}\right)^{2+s}|\mathbf{x}\cdot\vec{e}_{\varphi}|^{2}\right)*\rho_{a,b}\right)(y_{1}\vec{e}_{\varphi} + y_{2}\vec{e}_{\varphi}^{\perp}) \begin{cases} = V_{1}\left(\frac{R_{1}}{r_{\varphi}}\right)^{s}, \quad y_{1}\in[-r_{\varphi},r_{\varphi}]\\ > V_{1}\left(\frac{R_{1}}{r_{\varphi}}\right)^{s}, \quad y_{1}\notin[-r_{\varphi},r_{\varphi}]\end{cases}$$

 Integrated together, we see the following is constant on support

$$\left(|\mathbf{x}|^{-s}\Omega(\theta) + \tau_s \int_{-\pi}^{\pi} \left(\frac{R_1}{r_{\varphi}}\right)^{2+s} |\mathbf{x} \cdot \vec{e_{\varphi}}|^2 \tilde{\Omega}(\varphi) \,\mathrm{d}\varphi\right) * \rho_{a,b}$$

• If $\tilde{\Omega} \ge 0$ then this generated potential is larger outside because the integration is a positive linear combination

Part 3.2: Collapse to 1D for strong anisotropy

Collapse to 1D $W_{\alpha}(\mathbf{x}) = |\mathbf{x}|^{-s}(1 + \alpha \omega(\theta)) + |\mathbf{x}|^2$

• Assume ω achieves minimum at $\omega(\frac{\pi}{2}) = 0$

• **Theorem** (C.-Shu 22'): For 0 < s < 1, if ω satisfies the non-degeneracy condition

$$\omega(\theta) \ge c_{\omega} \left| \theta - \frac{\pi}{2} \right|^2, \quad \forall \theta \in [0, \pi].$$

then minimizers collapse to 1D vertical distribution for sufficiently large α



The non-degeneracy is necessary

Proof by comparison

- Lemma (C.-Shu 22'): there exists a smooth Ω_* such that the potential $W_*(\mathbf{x}) = |\mathbf{x}|^{-s} \Omega_*(\theta) + |\mathbf{x}|^2$ satisfies
 - $\hat{W}_*(\xi) \ge 0$ (LIC) $\longleftarrow W_*$
 - $W_* * \rho_{1D}$ achieves minimum on support
- If viewing W_* as an element in the family W_{α} , one has no 'gap' between ellipses and 1D vertical minimizer. In the logarithmic potential case, CMMSRV 20' considered exactly such a potential
- The theorem follows from a comparison similar to CMMSRV 20'

Part 3.3: Zigzag formation in between

Local expansion around 1D segment

• Theorem (C.-Shu 22'): for 0 < s < 1 and a 1D segment

 $\rho(\mathbf{x})$

 $\rho(\mathbf{x}) = \psi(x_2)\delta(x_1)$

the generated potential has the expansion

$$(W * \rho)(\epsilon, 0) - (W * \rho)(0, 0) = \frac{1}{2\tau_{2-s}} \tilde{\Omega}(0)\psi(0)\epsilon^{1-s} + O(\epsilon)$$

 $\tau_{2-s} < 0$

 The local stability of a 1D segment is related the negativity of the Fourier transform of W in the direction of its normal.

Local expansion around 1D segment

 $W_{\alpha}(\mathbf{x}) = |\mathbf{x}|^{-s} (1 + \alpha \omega(\theta)) + |\mathbf{x}|^2 \qquad \hat{W}_{\alpha}(\xi) = |\xi|^{-2+s} (c_s + \alpha \tilde{\omega}(\varphi))$

- Assume $\tilde{\omega}$ achieves the most negative value NOT at $\varphi = 0$ As α increases, the first "allowed" direction of 1D segment is not the vertical direction.
- This guarantees the appearance of zigzags.

 $0 \qquad \text{LIC, ellipses} \qquad \alpha_L \begin{array}{c} \text{guaranteed} \\ \text{zigzags} \end{array} \qquad \alpha_* \ 1 \text{D vertical minimizer} \qquad \alpha \\ \end{array}$



Remarks

- This framework can be generalized to higher dimensions (C.-Shu 23' in 3D)
- The logarithmic potentials can be derived as a limit $s \rightarrow 0^+$. Most results can be carried over. This generalizes the result in CMMSRV 20'.

- The set of ellipse-shaped distributions is closed under the associated Wasserstein-2 gradient flows. Long time convergence to the minimizer can be justified in the LIC case.
- Open question: $\omega(\theta) = \cos^2 \theta \sin^2 \theta$

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