Interaction-Driven Dynamics for Collective Behavior: Derivation, Model Hierarchies and Pattern Stability

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Outline

Problem & Motivation

- Minimization of the Interaction Energy
- Collective Behavior Models

2 Macroscopic Models: Repulsive-Attractive Potentials

- Steady States (Local) Minimizers
- Local Minimizers: Dimensionality of the support
- Geometry of support of d_{∞} -local minimizers
- Minimizers for Repulsive-Attractive Potentials



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Minimization of the Interaction Energy

Aggregation for particles - Continuum Model

One particle attracted/repelled by a fixed location x = a

 $\dot{X} = -\nabla U(X - a)$ $U(x) = U(-x), U(0) = 0, U \in C(\mathbb{R}^d, \mathbb{R}) \cap C^1(\mathbb{R}^d/\{0\}, \mathbb{R})$





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Multiple particles attracted by one another

$$\dot{X}_i = -\sum_{j \neq i} m_j \nabla U(X_i - X_j)$$



 $\rho(t, x) =$ density of particle at time t

$$v(x) = -\int_{\mathbb{R}^d} \nabla U(x-y) \ \rho(y) dy$$

So $v = -\nabla U * \rho$:

 $\begin{cases} \rho_t + \mathrm{div}\partial\rho v = 0\\ v = -\nabla U * \rho \end{cases}$

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$$\begin{cases} \rho_t + \operatorname{div} \rho v = 0\\ v = -\nabla U * \rho \end{cases}$$

 $U: \mathbb{R}^d \to \mathbb{R}$ "interaction potential" $\rho(t, x)$: density v(t, x): velocity field $x \in \mathbb{R}^d, t > 0$

> $-\nabla U: \mathbb{R}^d \to \mathbb{R}^d$ fattracting/repulsing field"





For which interaction repulsive/attractive potentials do we get convergence towards some nontrivial steady states? How can we find these stationary states and what are their properties?

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Formal Gradient Flow

Basic Properties

- Conservation of the center of mass.
- **2** Liapunov Functional: Gradient flow of

$$\mathcal{F}[\rho] = \frac{1}{2} \iint U(x - y) \ \rho(x) \ \rho(y) \ dxdy$$

with respect to the Wasserstein distance *W*₂. (C., McCann, Villani; RMI 2003, ARMA 2006).

The macroscopic equation can be rewritten as

$$\frac{\partial \rho}{\partial t}(t,x) = \operatorname{div}\left(\rho(t,x)\nabla\left[\frac{\delta \mathcal{F}}{\delta \rho}(t,x)\right]\right) \ .$$

with entropy dissipation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[\rho(t)] = -\int_{\mathbb{R}^2} \rho(t,x) \left| \nabla \frac{\delta \mathcal{F}}{\delta \rho}(t,x) \right|^2 \, dx \, .$$

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Minimization of the Interaction Energy

Minimization Problem

We want to find local minimizers of the total interaction energy

$$\mathcal{F}[\mu] := \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y) \, d\mu(x) d\mu(y) \, .$$

in some set of probability measures $\mathcal{P}(\mathbb{R}^d)$.

What is the right topology to talk about measures being close?

Recurrent Question in many fields:

- Statistical Mechanics & Crystallization: Typically very singular potentials at zero: Lennard-Jones.
- Semiconductors Astrophysics Chemotaxis: Macroscopic model obtained from Vlasov Equation under certain limits. Newtonian Potential.
- Economic Applications: Mean Field Games, Cournot-Nash Equilibria.
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3 Conclusions

Individual Based Models (Particle models)

Swarming = Aggregation of agents of similar size and body type generally moving in a coordinated way.

Highly developed social organization: insects (locusts, ants, bees ...), fish, birds, micro-organisms,... and artificial robots for unmanned vehicle operation.

Interaction regions between individuals^a

^aAoki, Helmerijk et al., Barbaro, Birnir et al.

- **Repulsion** Region: R_k .
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Nontrivial patterns? - Particle Simulations



Macroscopic Models: Repulsive-Attractive Potentials

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Steady States - (Local) Minimizers

Summary: Particle Simulations d = 2



Problem & Motivation	Macroscopic Models: Repulsive-Attractive Potentials	
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Steady States - (Local) Minimizers		
Spherical shell		

A spherical shell for some radius R is a stationary state for the aggregation equation for radial potentials.



Local Minimizers: Dimensionality of the support

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2

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Local Minimizers: Dimensionality of the support		
W_∞ -Topology		

$$W_{\infty}(\mu,\nu) = \inf_{\pi \in \Pi(\mu,\nu)} \sup_{(x,y) \in \operatorname{supp}(\pi)} |x-y|,$$

- It is a good topology since it is closer to linearization around equilibrium of dynamical systems.
- It is the coarser topology among Wasserstein distances since all of them are ordered.
- Then, a local minimizer in W_2 is a local minimizer in W_{∞} but not viceversa.

Basic Hypotheses:

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Euler-Lagrange Conditions

W_{∞} EL-Conditions

Assume that U satisfies (H1) and let μ be a local compactly supported minimizer of the energy $\mathcal{F}[\mu]$ in the W_{∞} ball or radius ε . Then any point $x_0 \in \text{supp}(\mu)$ is a local minimimum of $\psi = U * \mu$ in the sense that

 $\psi(x_0) \leq \psi(x)$ for a.e. $x \in B_{\varepsilon}(x_0)$.

Note that ε is uniform on the support of μ .

W₂ EL-Conditions

Under the same assumptions, if μ is a W_2 -local minimizer of the energy, then the potential ψ satisfy

- (i) $\psi(x) = (U * \mu)(x) = 2\mathcal{F}[\mu] \mu$ -a.e.
- (ii) $\psi(x) = (U * \mu)(x) \ge 2\mathcal{F}[\mu]$ for a.e. $x \in \mathbb{R}^d$.

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Regularity??

Mild versus Strong Repulsive potentials

Support is essentially 0-dimensional for b > 2.

Let $U \in C^2(\mathbb{R}^N)$ be a radially symmetric potential which behaves like $-|x|^b/b$ in a neighborhood of the origin with b > 2.

Then a local minimizer of the interaction energy \mathcal{F} with respect to W_{∞} cannot have a *s*-dimensional smooth components for any $1 \le s \le d$.

Dimension of the Support depends on 2 - d < b < 2.

Assume that μ is a local minimizer of the interaction energy \mathcal{F} with respect to W_{∞} such that U is radial with $U(x) \sim -|x|^b$ near zero and 2 - d < b < 2. If μ contains *s*-Haussdorff dimensional connected components in its support, then $s \geq 2 - b$.

(Balagué, C., Laurent, Raoul; ARMA 2013)

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Macroscopic Models: Repulsive-Attractive Potentials

Assume the following hypotheses on U hold.

(H1) $U \in C^2(\mathbb{R}^d)$ and U is radially symmetric.

- (H2) U is **bounded from below** and U(0) = 0.
- (H3) There exists R > 0 with U(x) < 0 for all |x| < R and $U(x) \ge 0$ for all $|x| \ge R$.
- (H4) Fix $\alpha > 2$. We write $\widetilde{U}(|x|) := U(x)$ and $\widetilde{U}_p(r) := \frac{\widetilde{U}(pr)}{p^{\alpha}}$ for any p > 0 and $r \ge 0$. There exists a constant C > 0 such that

$$egin{cases} \widetilde{U}_p(r) o - Cr^{oldsymbol{lpha}} \ \widetilde{U}_p'(r) o - Coldsymbol{lpha} r^{oldsymbol{lpha}-1} \ \widetilde{U}_p'(r) o - Coldsymbol{lpha} r^{oldsymbol{lpha}-1} \end{cases}$$
 as $p o 0$ for all $r \ge 0$.

Second variation of energy.- Let μ be a d_{∞} -local minimizer of E with $E(\mu) < +\infty$. There exists $\delta > 0$ such that for all $x_0 \in \text{supp}\mu$ we have

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y) \, \mathrm{d}\nu(x) \, \mathrm{d}\nu(y) \ge 0$$

for any measure ν with $\operatorname{supp}\nu \subset \operatorname{supp}\mu \cap B(x_0, \delta)$ and $\nu(\mathbb{R}^d) = 0$.

Macroscopic Models: Repulsive-Attractive Potentials

Assume the following hypotheses on U hold.

(H1) $U \in C^2(\mathbb{R}^d)$ and U is radially symmetric.

- (H2) U is **bounded from below** and U(0) = 0.
- (H3) There exists R > 0 with U(x) < 0 for all |x| < R and $U(x) \ge 0$ for all $|x| \ge R$.
- (H4) Fix $\alpha > 2$. We write $\widetilde{U}(|x|) := U(x)$ and $\widetilde{U}_p(r) := \frac{\widetilde{U}(pr)}{p^{\alpha}}$ for any p > 0 and $r \ge 0$. There exists a constant C > 0 such that

$$\begin{cases} \widetilde{U}_p(r) \to -Cr^{\boldsymbol{\alpha}} \\ \widetilde{U}'_p(r) \to -C\boldsymbol{\alpha}r^{\boldsymbol{\alpha}-1} \end{cases} \quad \text{as } p \to 0 \text{ for all } r \ge 0. \end{cases}$$

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Macroscopic Models: Repulsive-Attractive Potentials

Theorem.¹ Let μ be a W_{∞} -local minimizer of *E*. Then each point of supp μ is isolated; in particular μ is atomic.

Steps of proof.

• Suppose $0, x_1, -x_2 \in \text{supp } \mu \cap B(0, \delta)$. Choose $\nu_{\lambda} = -\delta_0 + \lambda \delta_{x_1} + (1-\lambda)\delta_{-x_2}$ in place of ν in the second variation and get, for an appropriate choice of λ ,

$$\sqrt{-U(x_1)} + \sqrt{-U(x_2)} \ge \sqrt{-U(x_1+x_2)}.$$

• Assume, by homogeneity, that $x_1 + x_2 = pe_1$, where e_1 is the first unit vector of the orthonormal base of \mathbb{R}^d , and p > 0 is a small rescaling parameter. From the above inequality, get

$$\sqrt{-U(x_1)} + \sqrt{-U(pe_1 - x_1)} \ge \sqrt{-U(pe_1)}.$$

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Geometry of support of $d \sim$ -local minimizers	

Macroscopic Models: Repulsive-Attractive Potentials

• Write $x_1 = p(te_1 + y)$, where $y \in \mathbb{R}^d$ with zero first coordinate, and, by homogeneity, $t \in [0, 1]$. Then, using that $|x_1| \leq pt + p|y|$ and $|pe_1 - x_1| \leq p(1-t) + p|y|$, and that, for any $x \in \mathbb{R}^d$ and p small enough, $\sqrt{-U(px)}$ is radially non-decreasing as a function of $x \in \mathbb{R}^d$, get

$$\sqrt{-\widetilde{U}(p(t+|y|))} + \sqrt{-\widetilde{U}(p((1-t)+|y|))} \ge \sqrt{-\widetilde{U}(p)}.$$

• Divide the inequality above by $p^{\alpha/2}$ and obtain

$$\sqrt{-\widetilde{U}_p(t+|y|)} + \sqrt{-\widetilde{U}_p((1-t)+|y|)} \ge \sqrt{-\widetilde{U}_p(1)}.$$

• By (H4) get, as $p \rightarrow 0$,

$$(t+|y|)^{\alpha/2} + ((1-t)+|y|)^{\alpha/2} \ge 1$$

Problem & Motivation		Macroscopic Models: Repulsive-Attractive Potentials
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Problem & Motivation

Macroscopic Models: Repulsive-Attractive Potentials

Conclusions

Geometry of support of d_{∞} -local minimizers

Macroscopic Models: Repulsive-Attractive Potentials

• For all $s \in [0, 1]$ and $z \in \mathbb{R}^d$, define

$$s_{\alpha}(s,z) = (s+|z|)^{\alpha/2} + ((1-s)+|z|)^{\alpha/2} - 1,$$

and define, for any two distinct points $v, v' \in \mathbb{R}^d$, the open set

$$S_{\alpha}(v,v') := \left\{ w \in \mathbb{R}^d \mid s_{\alpha}\left(\frac{|\pi w - v|}{|v - v'|}, \pi w - w\right) < 0 \right\},\$$

where π denotes the orthogonal projection on the segment [v, v'].

• What we have shown: for any $y_0, y_1 \in \text{supp } \mu$, asymptotically close, there cannot be a third point in $\text{supp } \mu \cap S_{\alpha}(y_0, y_1)$.

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Geometry of support of d_{∞} -local minimizers

Macroscopic Models: Repulsive-Attractive Potentials



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• For any two distinct points $v, v' \in \mathbb{R}^d$, define the open "double cone" with opening $\tau > 0$ by

$$C_{\tau}(v,v') := \left\{ w \in \mathbb{R}^{d} \mid \frac{\text{dist}(w, [v, v'])}{\min\{|\pi w - v|, |\pi w - v'|\}} < \tau \right\},\$$

where [v, v'] denotes the segment joining v to v' and π denotes the orthogonal projection on the segment [v, v'].

- Since α > 2, r → r^{α/2} is a convex function on [0, +∞), and so S_α(y₀, y₁) is a convex set. Therefore we can fit a double cone generated by y₀ and y₁ inside it.
- We can actually compute the opening $\gamma(\alpha)$ of the cone that fits in $S_{\alpha}(y_0, y_1)$ with maximal volume:

$$\gamma(\alpha) = \frac{1}{2^{\alpha/2 - 1}} - 1.$$

• Finish the proof by contradiction. Suppose y_0 is not an isolated point, then it can be approached by a sequence of points in $\text{supp}\mu$ in some direction. Therefore, using (H4) we know that, close enough to y_0 , one can find two points belonging to this sequence, say x_k and x_{k+1} , such that $x_{k+1} \in C_{\gamma(\alpha)}(y_0, x_k)$.

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Outline

2

Problem & Motivation

- Minimization of the Interaction Energy
- Collective Behavior Models

Macroscopic Models: Repulsive-Attractive Potentials

- Steady States (Local) Minimizers
- Local Minimizers: Dimensionality of the support
- Geometry of support of d_{∞} -local minimizers
- Minimizers for Repulsive-Attractive Potentials

3 Conclusions

Existence Global Minimizers

Non-HStable: Energy at infinity cost more than near the origin, i.e., the potential *U* satisfies

- (H5) There exists $\mu \in \mathcal{P}(\mathbb{R}^d)$ compactly supported such that $\mathcal{F}[\mu] < 0$.
- (H5) $\lim_{|x|\to\infty} U(x) \ge 0.$

Main Theorem

Assume that the radial potential U satisfies Hypotheses (H1), (H5), and is increasing outside a large ball. Then there exists a global minimiser for the energy \mathcal{F} . Furthermore, any such global minimiser has compact support.

(Cañizo, C., Patacchini; preprint 2014) Main ideas: Uniform repartition of the mass over the support.

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Key Estimate

By (H1) for *R* large enough:

$$E_R := \min \left\{ \mathcal{F}[\mu] \mid \mu \in \mathcal{P}_R(\mathbb{R}^d)
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Euler-Lagrange: for ρ_R -almost all $z \in \text{supp}\rho_R$ we have

$$\frac{1}{2}\int_{\mathbb{R}}U(z-x)\,\mathrm{d}\rho_R(x)=E_R.$$

Choose $A \in \mathbb{R}$ with $\frac{1}{2}U_{\min} \leq E_* < A < 0$ and r' > 0 with $U(x) \geq 2A$ for $|x| \geq r'$. Then for ρ_R -almost every z we have

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Problem & Motivation	Macroscopic Models: Repulsive-Attractive Potentials	
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Examples

Power-laws & Morse Potentials

Consider the following potentials for all $x \in \mathbb{R}^d$ and $C_A, C_R, \ell_A, \ell_R > 0$:

(i) (Power-law potential) $U(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b}$ with -d < b < a,

(ii) (Morse potential) $U(x) = C_R e^{-\frac{|x|}{\ell_R}} - C_A e^{-\frac{|x|}{\ell_A}}$ with either $\ell_A < \ell_R$ and $\frac{C_A}{C_R} < \left(\frac{\ell_R}{\ell_A}\right)^d$,

with the convention $\frac{|x|^0}{0} = \log |x|$.

Discrete To Continuum: Power-law Case

(C., Chipot, Huang; preprint 2014)

Discrete Setting: Find

$$I_N = \inf_{x \in (\mathbb{R}^d)^N} \mathcal{F}_N(x) \,,$$

with

$$\mathcal{F}_N(x_1,\cdots,x_N) = \sum_{i
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ight) \,.$$

Uniform Control of the support

Suppose that $1 \le b < a$. Then the diameter of any global minimizer of \mathcal{F}_N achieving the infimum I_N is bounded independently of N.

Key Idea: use Euler-Lagrange and a convexity argument for the repulsive potential to estimate the distance between the two particles the furthest away.

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Regularity of Local Minimizers

(H6) The function $U_a(x) := U(x) - V(x)$ with V being the Newtonian potential in dimension d satisfies:

 $\Delta U_a \in L^p_{loc}(\mathbb{R}^d)$ for some $p \in (d, \infty]$

with ΔU_a bounded below.

Main Theorem

Assume that the potential U satisfies Hypotheses (H1) and (H6). Then any μ compactly supported W_{∞} local minimizer of the energy \mathcal{F} is bounded uniformly, i.e., $\mu = \rho(x)d\mathcal{L}^d$ with $\rho \in L^{\infty}(\mathbb{R}^d)$.

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Obstacle Problem

Continuity of the potential

Assume that the potential *U* satisfies Hypotheses (H1) and (H3). Let μ be a W_{∞} local minimizer of *E*. Then the potential $\psi(x) := U * \mu(x)$ associated to μ is a continuous function in \mathbb{R}^N .

Implicit Obstacle Problem

For all $x_0 \in \text{supp}(\mu)$, the potential function ψ is equal, in $B_{\varepsilon}(x_0)$, to the unique solution of the obstacle problem

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$$\mu = -\Delta \psi + F.$$

Particular Case: Newtonian repulsion and quadratic confinement, the global minimizer is the characteristic of a ball with unit mass upto translations.

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- If the strength of the repulsion is stronger than or equal to Newtonian, they are bounded uniformly.
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