Minimizing Interaction Energies

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BIRS, Banff, Canada Day 2014

Outline

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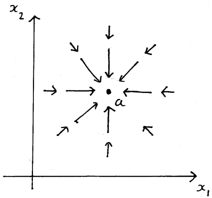
Aggregation for particles - Continuum Model

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

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

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 $\boxed{v = -\nabla U * \rho}$:

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

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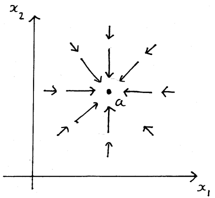

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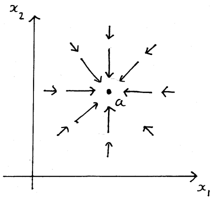

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Formal Gradient Flow

Basic Properties

1. **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

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

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.
- Fractional Diffusion: More singular than Newtonian repulsion but still locally integrable potentials. Levy Flights.
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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]

[a] Aoki, Helmerijk et al., Barbaro, Birnir et al.

- Repulsion Region: R_k.
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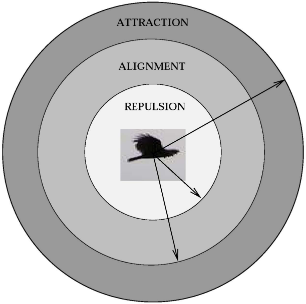

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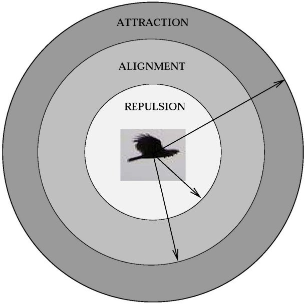

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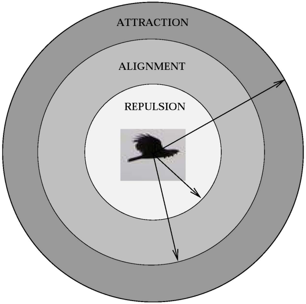
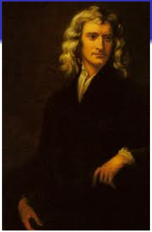


2nd Order Model: Newton's like equations



D'Orsogna, Bertozzi et al. model (PRL 2006):

$$\begin{cases} \dfrac{dx_i}{dt} = v_i, \\ m\dfrac{dv_i}{dt} = (\alpha - \beta\,|v_i|^2)v_i - \sum_{j\neq i} \nabla U(|x_i - x_j|). \end{cases}$$

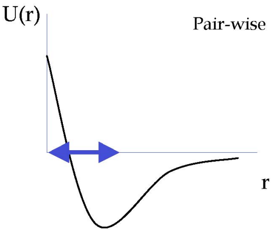
Model assumptions:

- Self-propulsion and friction terms determines an asymptotic speed of $\sqrt{\alpha/\beta}$.
- Attraction/Repulsion modeled by an effective pairwise potential $U(x)$.

$$U(r) = -C_A e^{-r/\ell_A} + C_R e^{-r/\ell_R}.$$

One can also use Bessel functions in 2D and 3D to produce such a potential.

$C = C_R/C_A > 1$, $\ell = \ell_R/\ell_A < 1$ and $C\ell^2 < 1$:



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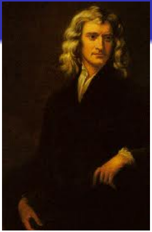

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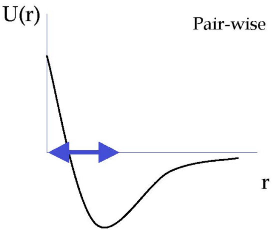

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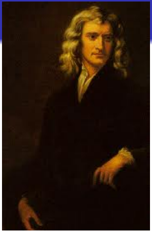

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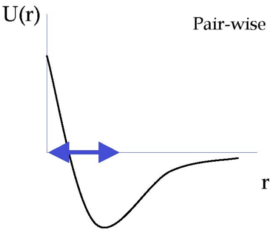

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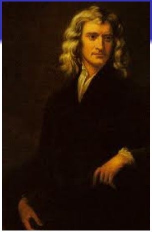

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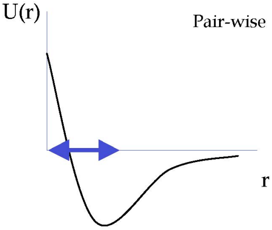
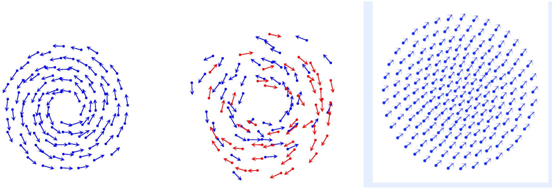


Model with an asymptotic speed

Typical patterns: milling, double milling or flocking:



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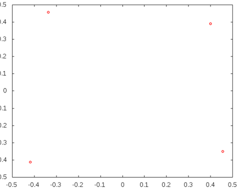
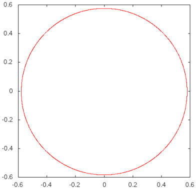
Particle Simulations $d = 2$

Potential $a = 4$, $b = 2.1$



Potential $a = 4$, $b = 1.85$



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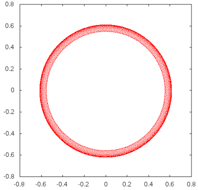
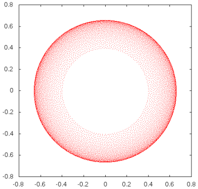
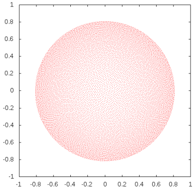


Potential $a = 4$, $b = 0.85$



Potential $a = 4$, $b = 0.05$



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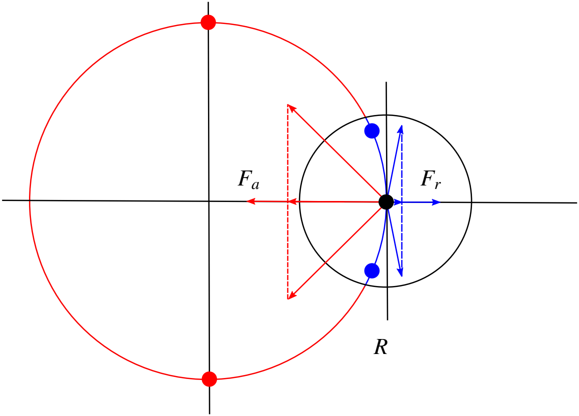
$$2 - d \leq b < a$$

Spherical shell

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



Outline

W_∞-Topology

The W_∞-distance is defined as the optimal maximal mass displacement given by

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

- 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:
(H1) U is a bounded from below lower semi-continuous function in $L^1_{loc}(\mathbb{R}^d)$.

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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

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

Note that ε is uniform on the support of μ.

W_2 EL-Conditions

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

(i) $\psi(x) = (U * \mu)(x) = 2\mathcal{F}[\mu]$ μ-a.e.

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

Regularity??

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

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

Note that ε is uniform on the support of μ.

W_2 EL-Conditions

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

(i) $\psi(x) = (U * \mu)(x) = 2\mathcal{F}[\mu]$ μ-a.e.

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Outline

Existence Global Minimizers

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

(H2) There exists $\mu \in \mathcal{P}(\mathbb{R}^d)$ compactly supported such that $\mathcal{F}[\mu] < 0$.

(H2) $\lim_{|x| \to \infty} U(x) \geq 0$.

Main Theorem

Assume that the radial potential U satisfies Hypotheses (H1), (H2), 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)
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Key Estimate

By (H1) for R large enough:

$$E_R := \min\left\{\mathcal{F}[\mu] \mid \mu \in \mathcal{P}_R(\mathbb{R}^d)\right\} \le E_* < 0$$

Euler-Lagrange: for ρ_R-almost all $z \in \operatorname{supp}\rho_R$ we have

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

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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)* $U(x) = C_A e^{-\frac{|x|}{\ell_A}} - C_R e^{-\frac{|x|}{\ell_R}}$ with $\ell_A < \ell_R$ 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; to appear in Phylosophical Transactions of the Royal Society)

Discrete Setting: Find

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

with

$$\mathcal{F}_N(x_1, \cdots, x_N) = \sum_{i \neq j}^{N} \left(\frac{|x_i - x_j|^a}{a} - \frac{|x_i - x_j|^b}{b} \right) \, .$$

Uniform Control of the support

Suppose that $1 \leq b < a$. 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

(H3) The function $U_a(x) := U(x) - V(x)$ with V being the Newtonian potential in dimension d satisfies:

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

with ΔU_a bounded below.

Main Theorem

Assume that the potential U satisfies Hypotheses (H1) and (H3). 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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Main ideas: Obstacle problems to obtain information out of the Euler-Lagrange conditions (Nash equilibria conditions).

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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

$$\begin{cases} \varphi \geq C_0, & \text{in } B_\varepsilon(x_0) \\ -\Delta\varphi \geq -F(x), & \text{in } B_\varepsilon(x_0) \\ -\Delta\varphi = -F(x), & \text{in } B_\varepsilon(x_0) \cap \{\varphi > C_0\} \\ \varphi = \psi, & \text{on } \partial B_\varepsilon(x_0), \end{cases}$$

where $C_0 = \psi(x_0)$ and $F(x) = \Delta U_a * \mu \in L^p_{loc}(\mathbb{R}^d)$. Furthermore, the density μ is given by

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

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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Conclusions

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