Minimization of an Energy Defined via an Attractive-Repulsive Interaction Potential

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joint work with R. Choksi (McGill) and R. Fetecau (Simon Fraser)

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A nonlocal aggregation model

Consider the aggregation equation

$$\rho_t - \nabla \cdot (\rho(\nabla K * \rho)) = 0 \text{ in } \mathbb{R}^N$$

where ρ=density of aggregation and K=interaction potential.

This equation arises in a number of applications: Granular media, self-assembly of nanoparticles, Ginzburg–Landau vortices, molecular dynamics simulations of matter, and in particular social aggregation models such as insect swarms, bird flocks, fish schools or bacteria colonies.

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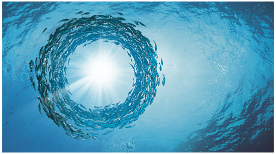
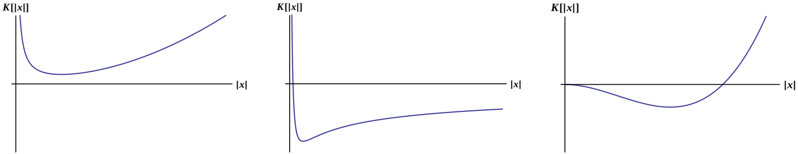


The repulsive-attractive interaction potential

The interaction potential is of the form

$$K(x) := \underbrace{\left(\frac{1}{q}|x|^q\right)}_{\substack{\text{attractive}\\\text{short-range}\\\text{interactions}}} + \underbrace{\left(-\frac{1}{p}|x|^p\right)}_{\substack{\text{repulsive}\\\text{long-range}\\\text{interactions}}}, \qquad x \in \mathbb{R}^N$$

for $-N < p < q$.



Examples of K with $-N < p < 0 < q$, $-N < p < q < 0$, and $0 < p < q$, resp.

Interaction energy

Minimize the energy

$$E[\rho] = \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} K(x-y)\rho(x)\rho(y)\, dxdy$$
$$= \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} \left(\frac{|x-y|^q}{q} - \frac{|x-y|^p}{p}\right)\rho(x)\rho(y)\, dxdy$$

The aggregation equation is the gradient flow of the energy with respect to the Wasserstein metric.

Indeed, the evolution equation can be written in the form

$$\partial_t \rho = \nabla \cdot \left(\rho \nabla \frac{\delta E[\rho]}{\delta \rho}\right).$$

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Particle models

Recent work by Bodnar/Velazquez, Balague, Bernoff, Bertozzi, Carrillo, Kolokolnikov, Laurent, Topaz,...: the gradient flow structure in the particle (individual-based) model describing the pairwise interaction of N particles in $\mathbb{R}^N$:

$$\frac{dX_i}{dt} = -\frac{1}{N} \sum_{\substack{i,j=1 \\ j \neq i}}^{N} \nabla_i K(X_i - X_j), \qquad i = 1 \dots N,$$

$X_i(t)$=the spatial location of the i-th individual at time t.

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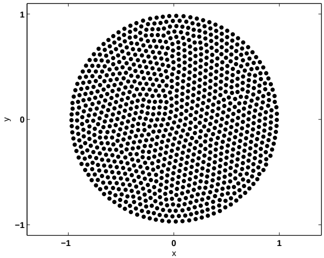
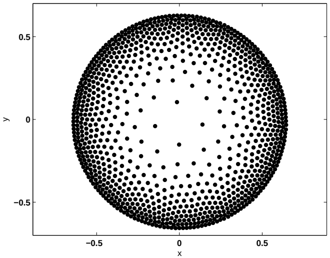
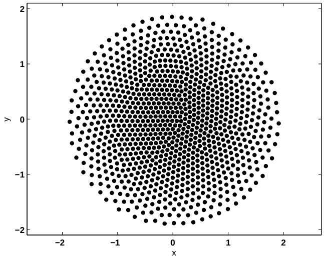
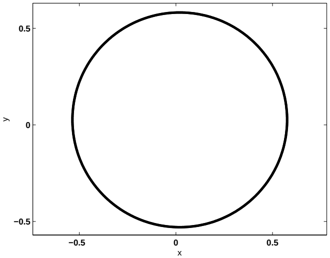




Newtonian repulsion with small positive attraction and large positive attraction





Below Newtonian repulsion, negative attraction and Positive repulsion, positive attraction

Back to the interaction energy

In the regime $-N < p < 0 < q$ or $-N < p < q < 0$ minimize the energy $E[\rho]$ over

- uniformly bounded
- radially symmetric
- non-negative

density functions $\rho \in L^1(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ satisfying a mass constraint

$$\|\rho\|_{L^1(\mathbb{R}^N)} = m > 0.$$

Even though uniform boundedness seems restrictive, previous work by Balague/Carrillo/Laurent/Raoul shows that when $p < 0$ and $N = 3$ minimizers cannot concentrate on sets of dimension less than 3.

Uniform boundedness is necessary to prevent concentrations. The energy does not bound any L^s-norm.

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We will use the direct method of the calculus of variations to prove the existence of minimizers. There are two key tools we need.

Lemma (Lions' concentration-compactness lemma)

For a sequence $\{\rho_n\}_{n\in\mathbb{N}} \subset L^1(\mathbb{R}^N)$ such that $\rho_n \geqslant 0$ and $\|\rho_n\|_{L^1} = m$ there exists a subsequence satisfying exactly one of the following three possibilities: tightness up to translation, vanishing or splitting.

Lemma (Convergence of energies)

Let ρ_n and ρ be admissible functions such that $\rho_n \rightharpoonup \rho$ weakly in $L^s(\mathbb{R}^N)$ for some $1 < s < \infty$. Then

$$\lim_{n\to\infty} \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} \frac{\rho_n(x)\rho_n(y)}{|x-y|^a}\,dxdy = \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} \frac{\rho(x)\rho(y)}{|x-y|^a}\,dxdy$$

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Existence of minimizers

Theorem

For any $m > 0$, and $-N < p < 0 < q$ or $-N < p < q < 0$ the energy $E[\rho]$ admits a minimizer over the uniformly bounded, radially symmetric non-negative density functions $\rho \in L^1(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ satisfying $\|\rho\|_{L^1(\mathbb{R}^N)} = m$.

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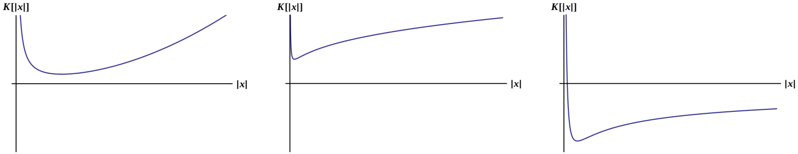

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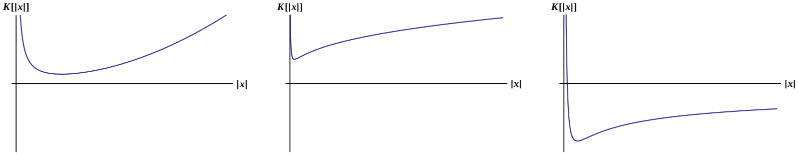

$-N < p < 0 < q$ case: We use the fact that $K(|x|) \nearrow \infty$ as $|x| \nearrow \infty$ to eliminate the possibilities of "vanishing" and "splitting" in the concentration-compactness lemma.

Next, tightness implies the existence of a weakly convergent subsequence and the fact that its weak limit is in the right class of admissible functions.

Finally the convergence lemma and the growth of K implies the weak lower semi-continuity.

$-N < p < q < 0$ case: In this case the minimum energy is negative and the character of the functional is different than before.

Look at the scaling

$$\rho_\lambda(x) = \frac{1}{\lambda^N}\rho_\lambda\left(\frac{x}{\lambda}\right).$$

ρ_λ is an admissible function for $\lambda \geqslant 1$.

Then the energy of ρ_λ is

$$E[\rho_\lambda] = \lambda^q \,\text{Attraction}(\rho) + \lambda^p \,\text{Repulsion}(\rho).$$

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Since Attraction$(\rho) < 0$ and Repulsion$(\rho) > 0$, taking λ large implies that $E[\rho_\lambda] < 0$. Thus the infimum is negative.

If "vanishing" occurs then one sees that

$$\liminf_{n\to\infty} \text{Attraction}(\rho_n) \geqslant 0.$$

Contradiction with the negativity of the infimum and the attraction part.

The scaling argument also provides a weak subadditivity condition (also used by Bedrossian for a different type of kernels):

$$\text{for} \quad m_1 > m_2 \quad \text{we have} \quad I_{m_1} < I_{m_2}.$$

Here $I_m =$ infimum with mass m.

This is used to eliminate "splitting;" hence, we can pass to a limit.

The weak lower semi-continuity again follows from the convergence lemma (this time directly).

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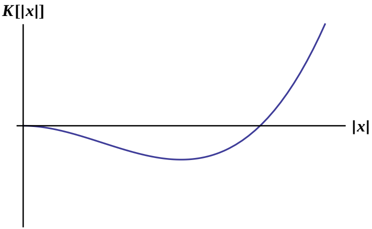
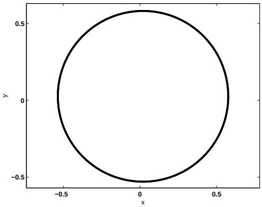
K does not have a singularity; hence, we need to allow concentrations on sets of dimension less than N.





Carrillo/DiFrancesco/Figalli/Laurent/Slepčev show existence of global-in-time weak measure solutions for

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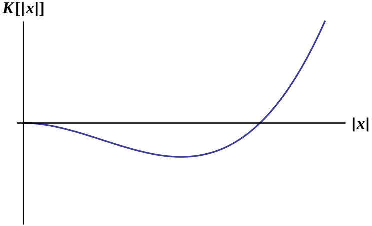

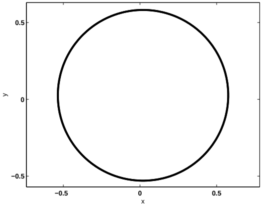

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For $q > p > 0$, define the energy over radially symmetric probability measures, $\mathcal{P}^r(\mathbb{R}^N)$:

$$E[\mu] = \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} \frac{|x-y|^q}{q} - \frac{|x-y|^p}{p}\, d\mu(x) d\mu(y).$$

Theorem

For any $q > p > 0$ the energy $E[\mu]$ admits a minimizer over $\mathcal{P}^r(\mathbb{R}^N)$.

Concentration-compactness lemma works also for measures: The growth of K and radial symmetry of measure $\Rightarrow$ "vanishing" and "splitting" does not occur.

A minimizing sequence is tight up to translation $\Rightarrow$ it has a weak-* convergent subsequence (Prokhorov's theorem) and the limit is in the admissible class.

Weak lower semi-continuity of the energy E follows since (a) K does not have a singularity at $x = 0$, (b) it is growing indefinitely with $|x|$, and (c) most of the mass of the weak-* limit lies in a ball.

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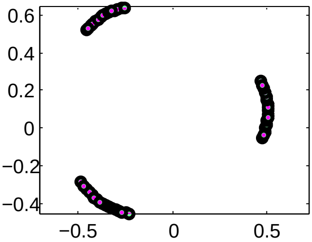

2D simulation with $q = 7$, $p = 1.5$

Particle simulations show non-radially symmetric steady states.

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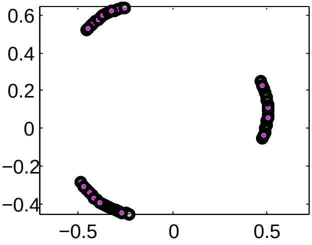

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In the regime $p < 0$ we conjecture:

Conjecture: Minimizers are radially symmetric.

Symmetric rearrangement type arguments don't apply immediately since K is decreasing. However, particle simulations do not reveal non-symmetric steady states.

$p < 0$ Case

We can give a weak characterization of critical points of $E[\rho]$ (weak formulation of Euler–Lagrange equation) as follows:

If ρ is a critical point of $E[\rho]$ then

$$\int_{\mathbb{R}^N}\int_{\mathbb{R}^N} |x-y|^q \rho(x)\rho(y)\, dxdy = \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} |x-y|^p \rho(x)\rho(y)\, dxdy .$$

Moreover, if ρ is a local minimizer then

$$\begin{aligned} \Lambda(x) \geqslant \mu \quad & \text{a.e. on the set} \quad \{x : \rho_0(x) = 0\} \\ \Lambda(x) = \mu \quad & \text{a.e. on the set} \quad \{x : \rho_0(x) > 0\} \end{aligned}$$

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Newtonian case $p = 2 - N$

Fetecau, Huang, Kolokolnikov consider the evolution equation when $p = 2 - N$. When $q > 2 - N$, they show the existence of a unique radially symmetric, bounded and compactly supported steady state.

In particular, when $q = 2$ the steady state consists of uniform density in a ball.

Bertozzi/Laurent/Leger show that these uniform densities are global attractors.

Looking at these steady states from a variational point of view we prove the following

Theorem

For any $m > 0$ and $M \geqslant \frac{m}{\omega_N}$, the function $\rho(x) = \dfrac{m}{\omega_N}\chi_{B(0,1)}(x)$ is the global minimizer of $E[\rho]$ when $q = 2$, $p = 2 - N$.

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Binary density version

$$\text{minimize} \quad \mathcal{E}(A) = \int_A \int_A K(x-y)\,dxdy$$

over radial sets A of finite measure subject to the constraint

$$|A| = m.$$

Following the calculations in Choksi/Sternberg we can find the criticality and stability conditions:

Criticality: If A a critical point of $\mathcal{E}(A)$, then

$$\Lambda(x) = \lambda \quad \text{for all } x \in \partial A,$$

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Stability: If A is a stable critical point, then for any smooth function ξ on ∂A satisfying the condition

$$\int_{\partial A} \xi(x)\, d\mathcal{H}^{N-1}_x = 0,$$

we have that

$$\int_{\partial A}\int_{\partial A} K(x-y)\xi(x)\xi(y)\, d\mathcal{H}^{N-1}_x d\mathcal{H}^{N-1}_y + \int_{\partial A} (\nabla\Lambda(x)\cdot\nu(x))\xi^2(x)\, d\mathcal{H}^{N-1}_x \geqslant 0,$$

where $\mathcal{H}^{N-1}$ denotes the $N-1$-dimensional Hausdorff measure, and ν denotes the unit normal on ∂A pointing out of A.

Theorem

For any $m > 0$ *let* $R := \left(\frac{m}{\omega_N}\right)^{1/N}$. *Then the ball* $B = B(0, R) \subset \mathbb{R}^N$ *is the global minimizer of* $\mathcal{E}(A)$ *when* $q = 2$ *and* $p = 2 - N$.

When $q = 2$ and $p = 2 - N$ an explicit calculation allows us to check criticality and stability.

Global minimality follows by looking at

$$\mathcal{E}(A) - \mathcal{E}(B)$$

and using the fact that the potential defined via the repulsive part solves

$$-\Delta\phi = C(\chi_A - \chi_B)$$

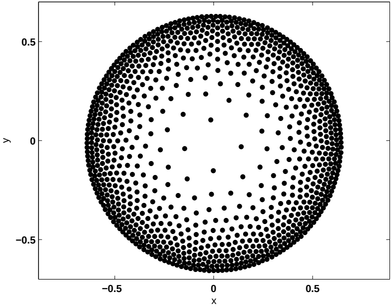
and is subharmonic on B.

Question: Do we see spherical annuli of constant density as critical points as we increase $q > 2$?

There does not exist a positive number $R > 0$ such that the spherical annulus

$$A := \{x \in \mathbb{R}^N \colon R < |x| < (m + R^N)^{1/N}\}$$

is a critical point of $\mathcal{E}(A)$ with $q > 2$ and $p = 2 - N$.



Particles accumulate at the boundary

Question: Do we ever see spherical annuli of constant density as critical points as we increase $q > 2$?

Answer: Yes, if we perturb the energy via Newtonian repulsion:

$$E_\delta[\rho] = \iint \left(\frac{|x-y|^q}{q} - \frac{|x-y|^p}{p} \right) \rho(x)\rho(y) + \delta \iint \frac{\rho(x)\rho(y)}{|x-y|^{N-2}}$$

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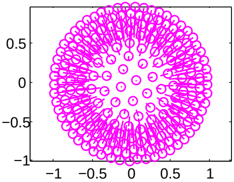

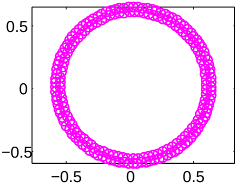

2D Particle simulations with $q = 3$, $p = 2$, and $\delta = 0.5$ and 0.0125

Kolokolnikov/Huang/Pavlovski show this using formal asymptotics.

Conjecture: This can be shown rigorously using Γ-convergence of $E_\delta[\rho]$ to $E[\mu]$ as $\delta \to 0$.

Thank you for your attention