Exact solutions and dynamics for the aggregation model with singular repulsion and long-range attraction

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Introduction

We consider a simple model of particle interaction,

\[
\frac{dx_j}{dt} = \frac{1}{N} \sum_{k=1,...,N}^{k\neq j} F(|x_j - x_k|) \frac{x_j - x_k}{|x_j - x_k|}, \quad j = 1 \ldots N
\] (1)


• Interaction force \( F(r) \) is of attractive-repelling type: the insects repel each other if they are too close, but attract each other at a distance.

• Mathematically \( F(r) \) is positive for small \( r \), but negative for large \( r \).

• Commonly, a \textit{Morse interaction force} is used:

\[
F(r) = \exp(-r) - G \exp(-r/L); \quad G < 1, \quad L > 1
\] (2)
• Under certain conditions on repulsion/attraction, the steady state typically consists of a bounded “particle cloud” whose diameter and is independent of $N$ in the limit $N \to \infty$. Then the continuum limit becomes

$$\rho_t + \nabla \cdot (\rho v) = 0; \quad v(x) = \int_{\mathbb{R}^n} F(|x - y|) \frac{x - y}{|x - y|} \rho(y) dy.$$ 

• Questions

1. Describe the equilibrium cloud shape in the limit $t \to \infty$

2. What about dynamics?
Morse force, h-stable vs. catastrophic

- If $GL^{n+1} > 1$, the system is catastrophic: doubling $N$ doubles the density but cloud volume is unchanged:

$$F(r) = e^{-r} - 0.5e^{-r/2}$$

- If $GL^{n+1} < 1$, the system is h-stable: doubling $N$ doubles the cloud volume: but density is unchanged:

$$F(r) = e^{-r} - 0.5e^{-r/1.2}$$
Morse force, explicit results

- Bernoff-Topaz, 2010: In one dimension, the steady states for the Morse force $F(r) = \exp(-r) - G \exp(-r/L)$ have the form

$$\rho(x) = \begin{cases} 
  a \cos(bx) + 1, & |x| < R \\
  0, & |x| > 0 
\end{cases}$$

where $a, b, c$ are related to $G, L$. 

(taken from Topaz+Bernoff, 2010 preprint)

- What about stability? Dynamics? 2D?
Bounded states of constant density

**Claim.** Suppose that

\[
F(r) = \frac{1}{r^{n-1}} - r, \quad \text{where } n \equiv \text{dimension}
\]

Then the aggregation model

\[
\rho_t + \nabla \cdot (\rho v) = 0; \quad v(x) = \int_{\mathbb{R}^n} F(|x - y|) \frac{x - y}{|x - y|} \rho(y) dy.
\]

admits a steady state of the form

\[
\rho(x) = \begin{cases} 
1, & |x| < R \\
0, & |x| > R
\end{cases} \quad v(x) = \begin{cases} 
0, & |x| < 1 \\
-ax, & |x| > 1
\end{cases}
\]

where \( R = 1 \) for \( n = 1, 2 \) and \( a = 2 \) in one dimension and \( a = 2\pi \) in two dimensions.
Constant density state in 2D, $F(r) - 1/r - r$: N=200 particles.
Proof for two dimensions

Define
\[ G(x) := \ln |x| - \frac{|x|^2}{2}; \quad M = \int_{\mathbb{R}^n} \rho(y)dy \]

Then we have:
\[ \nabla G = F(|x|) \frac{x}{|x|} \quad \text{and} \quad \Delta G(x) = 2\pi \delta(x) - 2. \]

so that
\[ v(x) = \int_{\mathbb{R}^n} \nabla_x G(x - y) \rho(y)dy. \]

Thus we get:
\[ \nabla \cdot v = \int_{\mathbb{R}^n} (2\pi \delta(x - y) - 2) \rho(y)dy \]
\[ = 2\pi \rho(x) - 2M \]
\[ = \begin{cases} 
0, & |x| < R \\
-2M, & |x| > R 
\end{cases} \]

The steady state satisfies \( \nabla \cdot v = 0 \) inside some ball of radius \( R \) with \( \rho = 0 \) outside such a ball but then \( \rho = M/\pi \) inside this ball and \( M = \int_{\mathbb{R}^n} \rho(y)dy = MR^2 \implies R = 1. \)
Dynamics in 1D with $F(r) = 1 - r$

Assume WLOG that

$$\int_{-\infty}^{\infty} x \rho(x) = 0; \quad M := \int_{-\infty}^{\infty} \rho(x) \, dx$$

Then

$$v(x) = \int_{-\infty}^{\infty} F(|x - y|) \frac{x - y}{|x - y|} \rho(y) \, dy$$

$$= \int_{-\infty}^{\infty} (1 - |x - y|) \text{sign}(x - y) \rho(y)$$

$$= 2 \int_{-\infty}^{x} \rho(y) \, dy - M(x + 1).$$

and continuity equations become

$$\rho_t + v \rho_x = -v_x \rho = (M - 2 \rho) \rho$$

Define the characteristic curves $X(t, x_0)$ by

$$\frac{d}{dt} X(t; x_0) = v; \quad X(0, x_0) = x_0$$
Then along the characteristics, we have $\rho = \rho(X, t)$;

$$\frac{d}{dt}\rho = \rho(M - 2\rho)$$

Solving we get:

$$\rho(X(t, x_0), t) = \frac{M}{2 + e^{-Mt}(M/\rho_0 - 2)}; \quad \rho(X(t, x_0), t) \to M/2 \text{ as } t \to \infty$$
Solving for characteristic curves

Let

\[ w := \int_{-\infty}^{x} \rho(y) dy \]

then

\[ v = 2w - M(x + 1); \quad v_x = 2\rho - M \]

and integrating \( \rho_t + (\rho v)_x = 0 \) we get:

\[ w_t + vw_x = 0 \]

Thus \( w \) is constant along the characteristics \( X \) of \( \rho \), so that characteristics \( \frac{d}{dt}X = v \) become

\[ \frac{d}{dt}X = 2w_0 - M(X + 1); \quad X(0; x_0) = x_0 \]
Summary for $F(r) = 1 - r$ in 1D:

$$X = \frac{2w_0(x_0)}{M} - 1 + e^{-Mt} \left( x_0 + 1 - \frac{2w_0(x_0)}{M} \right)$$

$$w_0(x_0) = \int_{-\infty}^{x_0} \rho_0(z)dz; \quad M = \int_{-\infty}^{\infty} \rho_0(z)dz$$

$$\rho(X, t) = \frac{M}{2 + e^{-tM}(M/\rho_0(x_0) - 2)}$$

Example: $\rho_0(x) = \exp\left(-x^2\right)/\sqrt{\pi}$; $M = 1$:
Global stability

In limit $t \to \infty$ we get:

$$X = \frac{2w_0}{M} - 1; \quad w_0 = 0 \ldots M; \quad \rho(X, \infty) = \frac{M}{2}$$

We have shown that as $t \to \infty$, the steady state is

$$\rho(x, \infty) = \begin{cases} M/2, & |x| < 1 \\ 0, & |x| > 1 \end{cases}$$

(3)

- This proves the global stability of (3)!

- Characteristics intersect at $t = \infty$; solution forms a shock at $x = \pm 1$ at $t = \infty$. 
Dynamics in 2D, \( F(r) = \frac{1}{r} - r \)

- Similar to 1D,

\[
\nabla \cdot v = 2\pi \rho(x) - 4\pi M;
\]

\[
\rho_t + v \cdot \nabla \rho = -\rho \nabla \cdot v = -\rho (\rho - 2M) 2\pi
\]

- Along the characteristics:

\[
\frac{d}{dt} X(t; x_0) = v; \quad X(0, x_0) = x_0
\]

we still get

\[
\frac{d}{dt} \rho = 2\pi \rho (2M - \rho);
\]

\[
\rho(X(t; x_0), t) = \frac{2M}{1 + \left( \frac{2M}{\rho(x_0)} - 1 \right) \exp(-4\pi M t)} \quad (4)
\]

- Continuity equations yield:

\[
\rho(X(t; x_0), t) \det \nabla_{x_0} X(t; x_0) = \rho_0(x_0)
\]
• Using (4) we get

$$\det \nabla_{x_0} X(t; x_0) = \frac{\rho_0(x_0)}{2M} + \left( 1 - \frac{\rho_0(x_0)}{2M} \right) \exp (-4\pi M t) .$$

• If $\rho$ is radially symmetric, characteristics are also radially symmetric, i.e.

$$X(t; x_0) = \lambda (|x_0|, t) x_0$$

then

$$\det \nabla_{x_0} X(t; x_0) = \lambda(t; r) (\lambda(t; r) + \lambda_r(t; r)r) , \quad r = |x_0|$$

so that

$$\lambda^2 + \lambda_r \lambda r = \frac{\rho_0(x_0)}{2M} + \left( 1 - \frac{\rho_0(x_0)}{2M} \right) \exp (-4\pi M t)$$

$$\lambda^2 r^2 = \frac{1}{M} \int_0^r s \rho_0(s) ds + 2 \exp (-4\pi M t) \int_0^r s \left( 1 - \frac{\rho(s)}{2M} \right) ds$$

So characteristics are fully solvable!!

• This proves global stability in the space of radial initial conditions $\rho_0(x) = \rho_0(|x|)$.

• More general global stability is still open.
The force \( F(r) = \frac{1}{r} - rq^{-1} \) in 2D

- If \( q = 2 \), we have explicit ode and solution for characteristics.

- For other \( q \), no explicit solution is available but we have **differential inequalities**:

  Define
  \[
  \rho_{\text{max}} := \sup_x \rho(x, t); \quad R(t) := \text{radius of support of } \rho(x, t)
  \]

  Then
  \[
  \frac{d\rho_{\text{max}}}{dt} \leq (aR^{q-2} - b\rho_{\text{max}})\rho_{\text{max}}
  \]
  \[
  \frac{dR}{dt} \leq c\sqrt{\rho_{\text{max}}} - dR^{q-1};
  \]

  where \( a, b, c, d \) are some [known] positive constants.

- It follows that if \( R(0) \) is sufficiently big, then \( R(t), \rho_{\text{max}}(t) \) remain bounded for all \( t \). [using bounding box argument]

- **Theorem**: For \( q \geq 2 \), there exists a bounded steady state [uniqueness??]
Inverse problem: Custom-designer kernels: 1D

**Theorem.** In one dimension, consider a radially symmetric density of the form

\[
\rho(x) = \begin{cases} 
    b_0 + b_2 x^2 + b_4 x^4 + \ldots + b_{2n} x^{2n}, & |x| < R \\
    0, & |x| \geq R
\end{cases}
\]  

(5)

Define the following quantities,

\[
m_{2q} := \int_0^R \rho(r) r^{2q} dr.
\]  

(6)

Then \(\rho(r)\) is the steady state corresponding to the kernel

\[
F(r) = 1 - a_0 r - \frac{a_2}{3} r^3 - \frac{a_4}{5} r^5 - \ldots - \frac{a_{2n}}{2n+1} r^{2n+1}
\]  

(7)

where the constants \(a_0, a_2, \ldots, a_{2n}\), are computed from the constants \(b_0, b_2, \ldots, b_{2n}\) by solving the following linear problem:

\[
b_{2k} = \sum_{j=k}^{n} a_{2j} \binom{2j}{2k} m_{2(j-k)}, \quad k = 0 \ldots n.
\]  

(8)
Example: custom kernels 1D

**Example 1:** $\rho = 1 - x^2, \ R = 1, \text{ then } F(r) = 1 - 9/5r + 1/2r^3$.

**Example 2:** $\rho = x^2, \ R = 1, \text{ then } F(r) = 1 + 9/5r - r^3$.

**Example 3:** $\rho = 1/2 + x^2 - x^4, \ R = 1; \text{ then } F(r) = 1 + \frac{209425}{336091}r - \frac{4150}{2527}r^3 + \frac{6}{19}r^5$. 
Theorem. In two dimensions, consider a radially symmetric density $\rho(x) = \rho(|x|)$ of the form

$$\rho(r) = \begin{cases} b_0 + b_2r^2 + b_4r^4 + \ldots + b_{2n}r^{2n}, & r < R \\ 0, & r \geq R \end{cases} \quad (9)$$

Define the following quantities,

$$m_{2q} := \int_0^R \rho(r)r^{2q}dr. \quad (10)$$

Then $\rho(r)$ is the steady state corresponding to the kernel

$$F(r) = \frac{1}{r} - \frac{a_0}{2}r - \frac{a_2}{4}r^3 - \ldots - \frac{a_{2n}}{2n+2}r^{2n+1} \quad (11)$$

where the constants $a_0, a_2, \ldots, a_{2n}$, are computed from the constants $b_0, b_2, \ldots, b_{2n}$ by solving the following linear problem:

$$b_{2k} = \sum_{j=k}^{n} a_{2j} \left( \begin{array}{c} j \\ k \end{array} \right)^2 m_{2(j-k)+1}, \quad k = 0 \ldots n. \quad (12)$$

This system always has a unique solution for provided that $m_0 \neq 0$. 
Numerical simulations, 1D

- First, use standard ODE solver to integrate the corresponding discrete particle model,
  \[
  \frac{dx_j}{dt} = \frac{1}{N} \sum_{k=1, k \neq j}^{N} F(|x_j - x_k|) \frac{x_j - x_k}{|x_j - x_k|}, \ j = 1 \ldots N.
  \]

- How to compute \( \rho(x) \) from \( x_i \)? [Topaz-Bernoff, 2010]
  - Use \( x_i \) to approximate the cumulative distribution, \( w(x) = \int_{-\infty}^{x} \rho(z)dz \).
  - Next take derivative to get \( \rho(x) = w'(x) \)

[Figure taken from Topaz+Bernoff, 2010 preprint]
Numerical simulations, 2D

- Solve for \( x_i \) using ODE particle model as before \([2N \text{ variables}]\)

- Use \( x_i \) to compute **Voronoi diagram**;

- Estimate \( \rho(x_j) = 1/a_j \) where \( a_j \) is the area of the voronoi cell around \( x_j \).

- Use **Delanay triangulation** to generate smooth mesh.

- **Example:** Take

  \[
  \rho(r) = \begin{cases} 
  1 + r^2, & r < 1 \\
  0, & r > 0 
  \end{cases}
  \]

  Then by Custom-designed kernel in 2D is:

  \[
  F(r) = \frac{1}{r} - \frac{8}{27} r - \frac{r^3}{3}.
  \]

  Running the particle method yeids...
Numerical solutions for radial steady states for $F(r) = \frac{1}{r} - r^{q-1}$

- Radial steady states of radius $R$ satisfy $\rho(r) = 2q \int_0^R (r'\rho(r')I(r, r')dr'$
  where $c(q)$ is some constant and $I(r, r') = \int_0^\pi (r'^2 + r'^2 - 2rr'\sin \theta)^{q/2-1}d\theta$.

- To find $\rho$ and $R$, we adjust $R$ until the operator $\rho \rightarrow c(q) \int_0^R (r'\rho(r')K(r, r')dr'$ has eigenvalue 1; then $\rho$ is the corresponding eigenfunction.

![Graph showing the behavior of $\rho_q$ for different values of $q$.]
Discussions/open problems

- We found bound states of **constant density with** $F(r) = r^{1-n} - r$.
  - May be of relevance for biology (minimizes overcrowding)

- Can we get explicit results for Morse force in 2D?
  - To get explicit results in $2D$, we need that $F(r) \sim 1/r$ as $r \to 0$.
  - Morse force looks like $F(r) \sim \text{const.}$ as $r \to 0$. This is a more “difficult” singularity in 2D.

- Open question: **global stability** for $F(r) = r^{1-n} - r$? [can show for $n = 1$ or for radial initial conditions if $n \geq 2$.]

- Open question: Uniqueness of (radial) steady states for $F(r) = r^{1-n} - r^{q-1}$, $q \neq 2$? [can show it is bounded for all $q$; can show uniqueness if $q = 2$]

- What about $q < 2$?

- Most of the results generalize to $n$ dimensions.

- This talk is downloadable from my website (preprint will be available by spring),
  http://www.mathstat.dal.ca/~tkolokol/papers