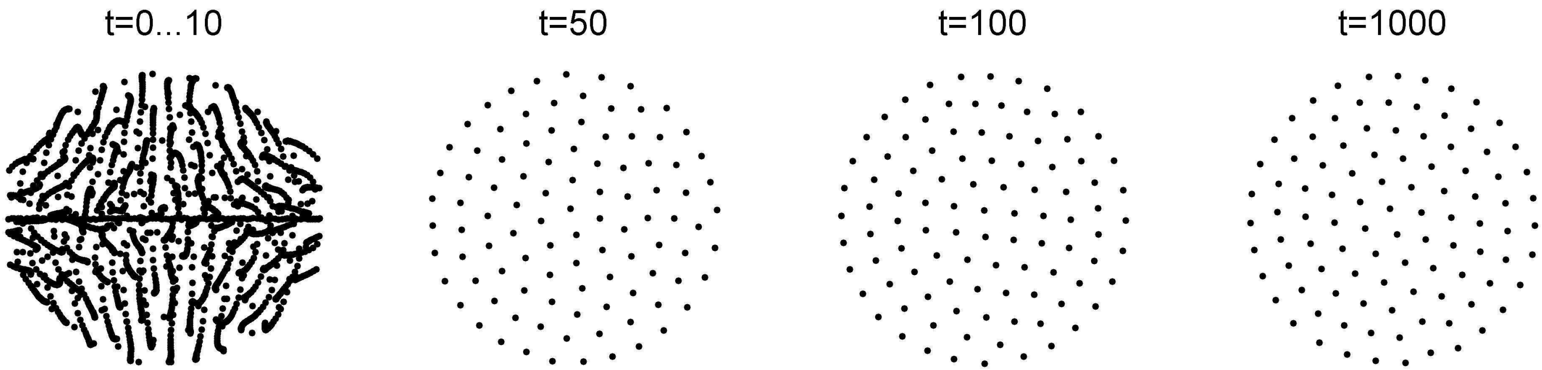
Exact solutions and dynamics for the aggregation model with singular repulsion and long-range attraction



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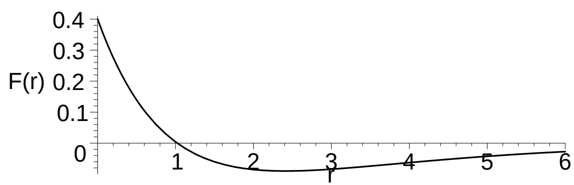
Introduction

We consider a simple model of particle interaction,

$$\frac{dx_j}{dt} = \frac{1}{N} \sum_{\substack{k=1\ldots N \\ k\neq j}} F\left(|x_j - x_k|\right) \frac{x_j - x_k}{|x_j - x_k|}, \quad j = 1\ldots N \qquad (1)$$

- Models insect aggregation [Edelstein-Keshet et al, 1998] such as locust swarms [Topaz et al, 2008]; robotic motion [Gazi, Passino, 2004].
- Interaction force $F\left(r\right)$ 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 ***Morse interaction force*** is used:

$$F(r) = \exp(-r) - G\exp(-r/L); \quad G < 1, L > 1 \qquad (2)$$



- 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

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

- Questions

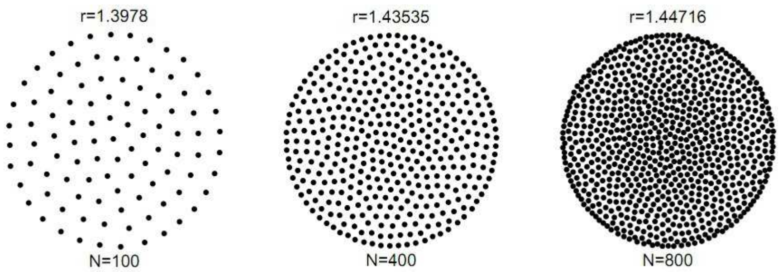
  1. Describe the equilibrium cloud shape in the limit $t \to \infty$

  2. What about dynamics?

Morse force, h-stable vs. catastrophic

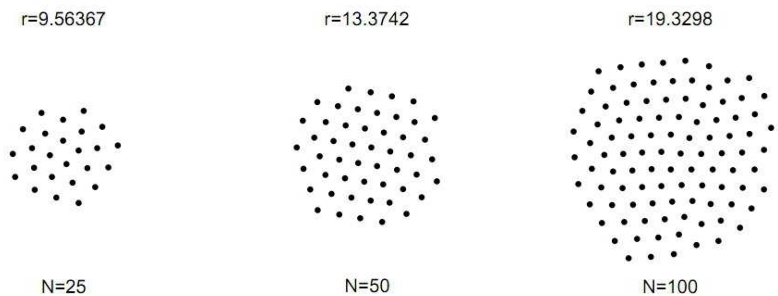
- If $GL^{n+1} > 1$, the system is ***catastrophic:*** doubling N doubles the density but cloud volume is unchanged:

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



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

$$F(r) = e^{-r} - 0.5e^{-r/1.2}$$

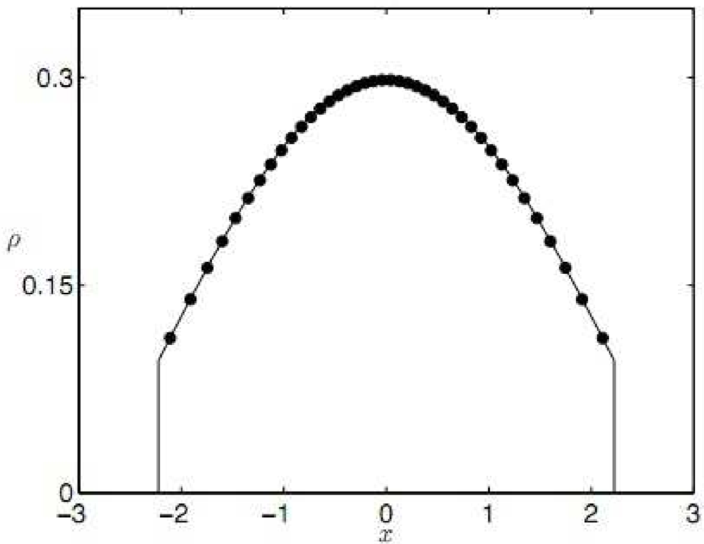


Morse force, explicit results

- 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

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

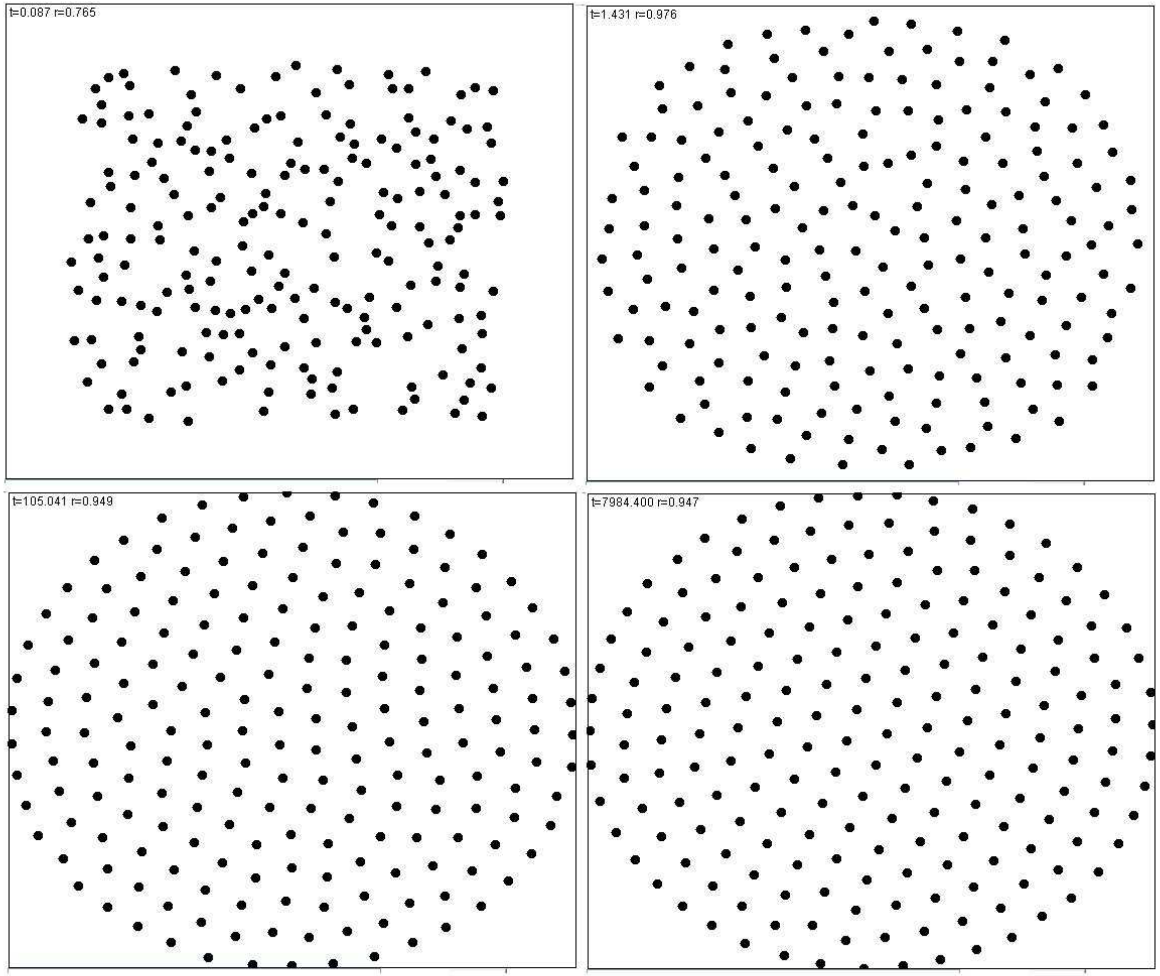
Then the aggregation model

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

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:

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

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

$$\begin{aligned} v(x) &= \int_{-\infty}^{\infty} F(|x-y|) \frac{x-y}{|x-y|} \rho(y) dy \\ &= \int_{-\infty}^{\infty} (1 - |x-y|) \operatorname{sign}(x-y) \rho(y) \\ &= 2 \int_{-\infty}^{x} \rho(y) dy - M(x+1). \end{aligned}$$

and continuity equations become

$$\begin{aligned} \rho_t + v\rho_x &= -v_x \rho \\ &= (M - 2\rho)\, \rho \end{aligned}$$

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

$$\frac{d}{dt} X(t; x_0) = v; \qquad X(0, x_0) = x_0$$

Then along the characteristics, we have $\rho = \rho(X, t)$;

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

Solving we get:

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

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 ρ, so that characteristics $\frac{d}{dt}X = v$ become

$$\frac{d}{dt}X = 2w_0 - M(X+1); \quad X(0; x_0) = x_0$$

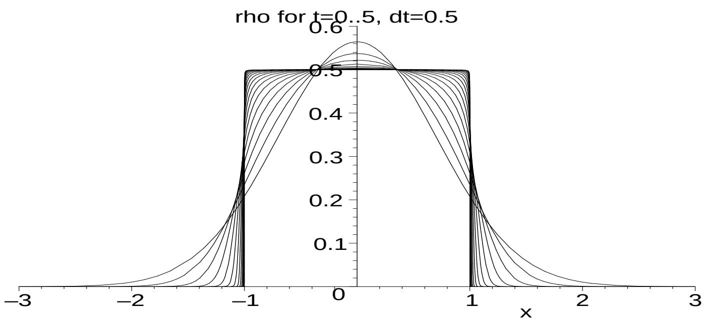
Summary for $F(r) = 1 - r$ in 1D:

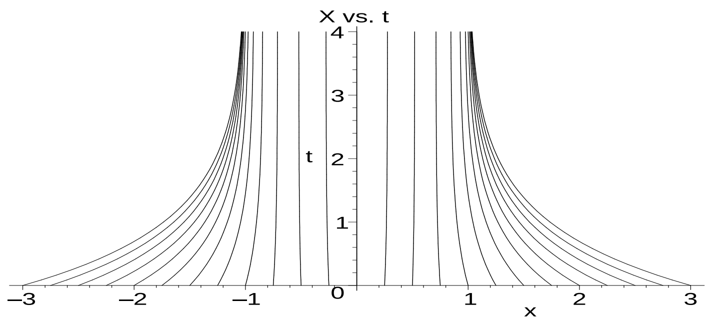
$$X = \frac{2w_0(x_0)}{M} - 1 + e^{-Mt}\left(x_0 + 1 - \frac{2w_0(x_0)}{M}\right)$$

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

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

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





Global stability

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

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

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

$$\rho(x,\infty) = \begin{cases} M/2, & |x| < 1 \\ 0, & |x| > 1 \end{cases} \qquad (3)$$

- 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,

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

$$\begin{aligned} \rho_t + v \cdot \nabla\rho &= -\rho\nabla \cdot v \\ &= -\rho\,(\rho - 2M)\,2\pi \end{aligned}$$

- Along the characterisitics:

$$\frac{d}{dt}X(t; x_0) = v; \qquad X(0, x_0) = x_0$$

we still get

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

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

- 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

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

- If ρ is **radially symmetric**, characteristics are also radially symmetric, i.e.

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

then

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

so that

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

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

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 $F(r) = \frac{1}{r} - r^{q-1}$ 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

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

  Then

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

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

- It follows that if $R(0)$ is sufficiently big, then $R(t), \rho_{\max}(t)$ 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, conisder a radially symmetric density of the form

$$\rho(x) = \begin{cases} b_0 + b_2 x^2 + b_4 x^4 + \ldots + b_{2n} x^{2n}, & |x| < R \\ 0, \quad |x| \geq R \end{cases} \tag{5}$$

Define the following quantities,

$$m_{2q} := \int_0^R \rho(r) r^{2q} dr. \tag{6}$$

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

$$F(r) = 1 - a_0 r - \frac{a_2}{3} r^3 - \frac{a_4}{5} r^5 - \ldots - \frac{a_{2n}}{2n+1} r^{2n+1} \tag{7}$$

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:

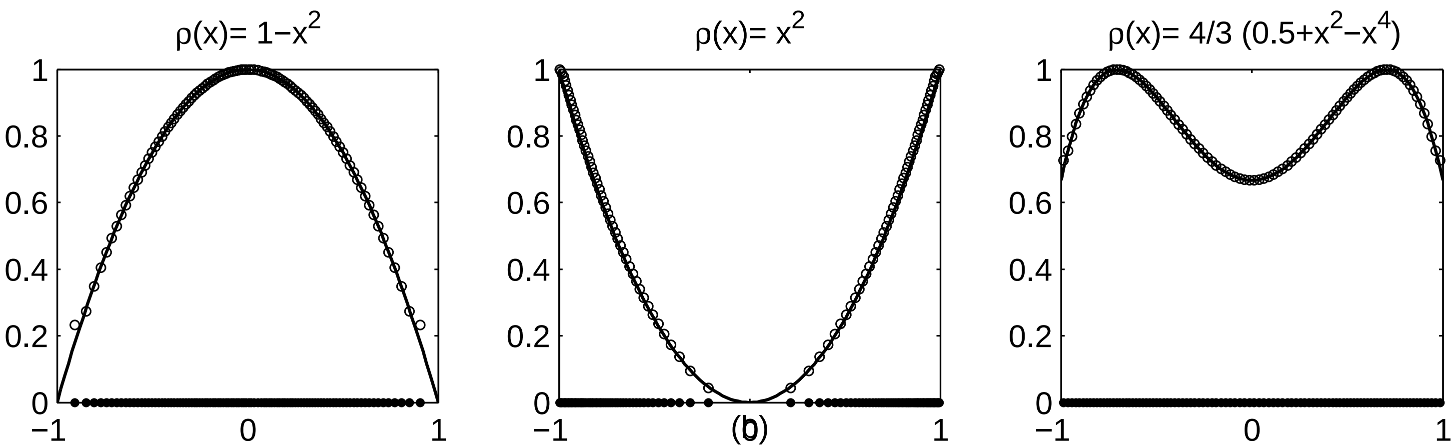
$$b_{2k} = \sum_{j=k}^{n} a_{2j} \begin{pmatrix} 2j \\ 2k \end{pmatrix} m_{2(j-k)}, \qquad k = 0 \ldots n. \tag{8}$$

Example: custom kernels 1D

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

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

Example 3: $\rho = 1/2 + x^2 - x^4, \;\; R = 1$; then $F(r) = 1 + \frac{209425}{336091}r - \frac{4150}{2527}r^3 + \frac{6}{19}r^5$.



Ex.1 Ex.2 Ex.3

Inverse problem: Custom-designer kernels: 2D

Theorem. In **two dimensions**, conisder a radially symmetric density $\rho(x) = \rho(|x|)$ of the form

$$\rho(r) = \begin{cases} b_0 + b_2 r^2 + b_4 r^4 + \ldots + b_{2n} r^{2n}, & r < R \\ 0, & r \geq R \end{cases} \tag{9}$$

Define the following quantities,

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

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

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

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:

$$b_{2k} = \sum_{j=k}^{n} a_{2j} \begin{pmatrix} j \\ k \end{pmatrix}^2 m_{2(j-k)+1}; \quad k = 0 \ldots n. \tag{12}$$

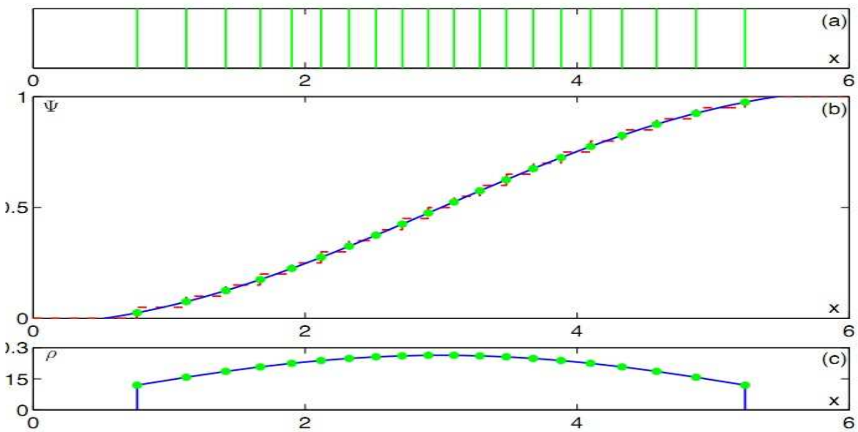
This system always has a unique solution for provided that $m_0 \neq 0$.

Numerical simulations, 1D

- First, use standard ODE solver to integrate the corresponding discrete particle model,

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

- How to compute $\rho(x)$ from x_i? [Topaz-Bernoff, 2010]
  - Use x_i to approximate the cumulitive 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

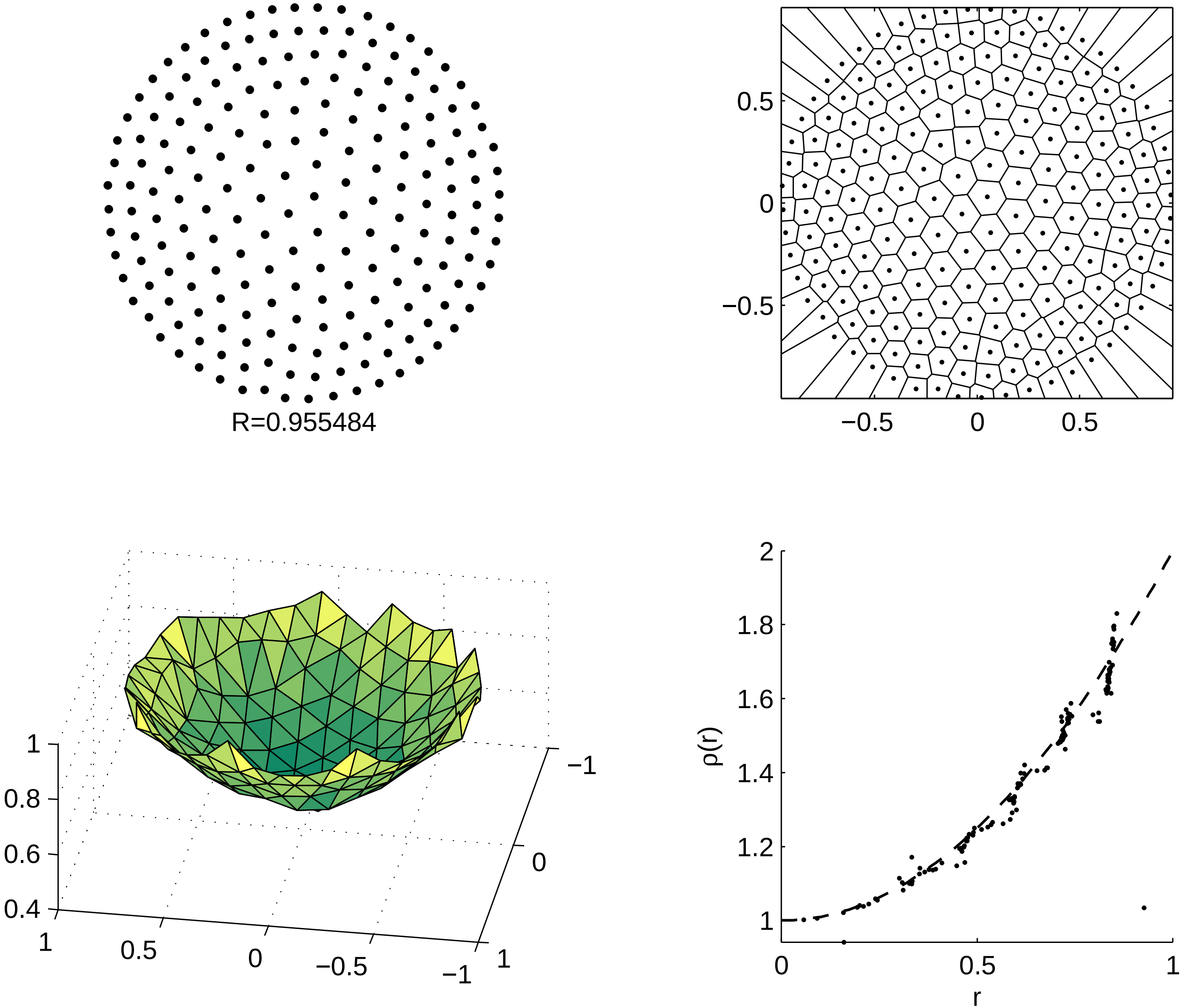
- Solve for x_i using ODE particle model as before [$2N$ variables]
- Use x_i to compute **Voronoi diagram**;
- Estimate $\rho(x_j) = 1/a_j$ where a_j is the area of the voronoi cell around x_j.
- Use **Delanay triangulation** to generate smooth mesh.
- **Example:** Take

$$\rho(r) = \begin{cases} 1 + r^2, r < 1 \\ 0, \quad r > 0 \end{cases}$$

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...

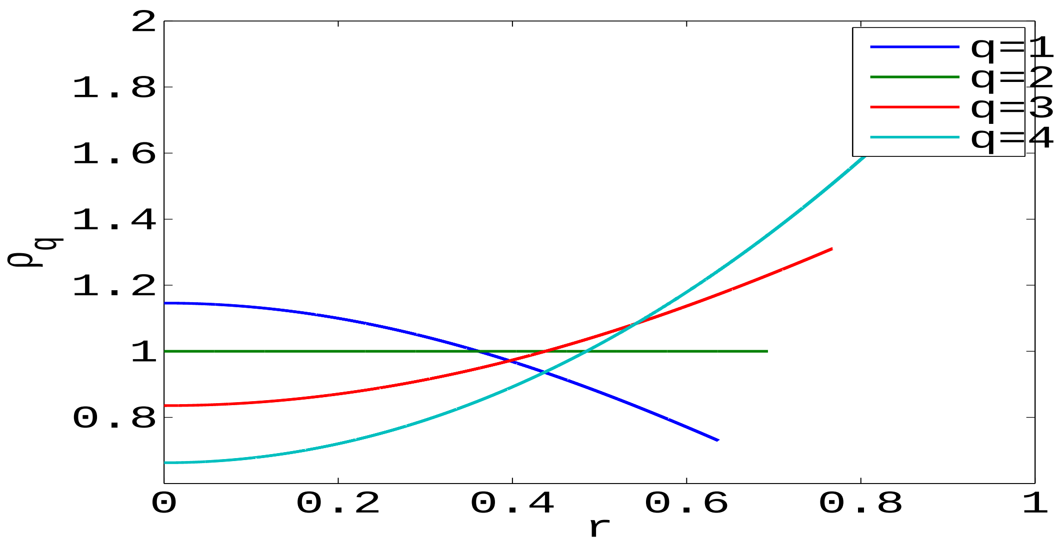

R=0.955484
0.5
0
−0.5
−0.5
0
0.5
1
0.8
0.6
0.4
1
0.5
0
−0.5
−1
−1
0
1
2
1.8
1.6
1.4
1.2
1
ρ(r)
0
0.5
1
r

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



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 $F(r) \sim const.$ 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`