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

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Outline

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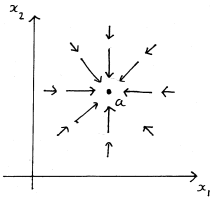
Aggregation for particles - Continuum Model

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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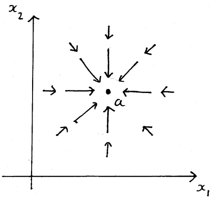

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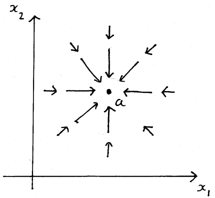

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Formal Gradient Flow

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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Sliding down in a Energy Landscape

Finite Dimensional Gradient flows

A *gradient flow* in $\mathbb{R}^d$ defined by an energy $\mathcal{F}$ is given by

$$\frac{dx_t}{dt} = -\nabla\mathcal{F}(x_t)\,.$$

It is the continuous version of the *steepest descent* on the energy landscape determined by $\mathcal{F}$ given by the implicit Euler scheme: given a time step Δt and an approximation to the solution at time $t_k = k\Delta t$, we find the approximation at time t_{k+1} by solving

$$x_{k+1} = x_k - \Delta t \nabla\mathcal{F}(x_{k+1})\,.$$

which is equivalent under convexity conditions to the following variational problem: Solve

$$x_{k+1} = \arg\min_{x\in\mathbb{R}^d} \left\{ \frac{1}{2\,\Delta t}|x - x_k|^2 + \mathcal{F}(x) \right\}$$

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JKO scheme (Jordan-Kinderlehrer-Otto)

A discrete time approximation of the PDE is obtained by solving a sequences of variational problem.

- Choose a time step Δt.
- Solve

$$\rho_{k+1} = \arg \min_{\rho \in \mathcal{P}_2^o(\mathbb{R}^d)} \left\{ \frac{1}{2\,\Delta t} W_2^2(\rho, \rho_k) + \mathcal{F}(\rho) \right\}$$

- As $\Delta t \to 0$ it converges to the solution of a weak form of

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

The convergence for smooth C^1 potentials U with at most quadratic growth at infinity given in "Gradient Flow in Metric Spaces" book by Ambrosio, Gigli, Savaré, 2005.

Is this theory with initial data measures really necessary?

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Is this theory with initial data measures really necessary?

How to deal with concentrations?

Let $U(x) = k(|x|)$ be a radial fully attractive potential with its only possible singularity located at zero such that

No-Osgood condition: $$\int_0^L \frac{dr}{k'(r)} < +\infty,$$

Then we are doomed to deal with concentrations in finite time.

- Given an initial condition in $L^1 \cap L^\infty$ (Bertozzi, C., Laurent; Nonlinearity 2009) or in $L^1 \cap L^p$ for $p > d/(d-1)$ (Bertozzi, Laurent, Rosado; CPAM 2011), the solutions blow up in finite time.
- Assume additionally that U is λ-convex: $U(x) - \frac{\lambda}{2}|x|^2$ is convex, then one can construct a well-posedness theory for measures going over the blow-up time in a unique way (C., Di Francesco, Figalli, Laurent, Slepcev; Duke MJ 2012). This assumption restrict the possible singularities at the origin, $U(x) \simeq |x|^\alpha$ locally at 0, with $1 \le \alpha < 2$, for instance.
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Internal Energy

$E\colon \mathcal{P}(\mathbb{R}^d) \to \mathbb{R} \cup \{-\infty, +\infty\}$ by

$$E(\rho) = \begin{cases} \int_{\mathbb{R}} H(\rho(x))\,\mathrm{d}x \text{ if } \rho \in \mathcal{P}_{ac,2}(\mathbb{R}^d) \\ +\infty \qquad \text{otherwise} \end{cases},$$

where $H : [0, \infty) \to \mathbb{R}$ is the density of *internal energy* satisfying $H(0) = 0$.

Let us consider N particles in $\mathbb{R}^d$ denoted by $x_N := (x_{1,N}, \ldots, x_{N,N}) \in \mathbb{R}^{Nd}$, where N is a positive integer. For all $i \in \{1, \ldots, N\}$, let us write $B_{i,N} := B(x_{i,N}, R_{i,N})$ the open ball of centre $x_{i,N}$ and radius

$$R_{i,N} = \frac{1}{2} \min_{j \neq i} |x_{i,N} - x_{j,N}|.$$

For these N particles consider

$$\rho_N = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{|B_{i,N}|} \chi_{B_{i,N}},$$

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Approximated Internal Energy

Given

$$\mathcal{A}_N(\mathbb{R}^d) = \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) \text{ such that } \exists x_N \in \mathbb{R}^{Nd}, \mu = \delta_{x_N} \right\}.$$

The discrete energy $E_N : \mathcal{A}_N(\mathbb{R}^d) \to \mathbb{R} \cup \{-\infty, +\infty\}$ by

$$E_N(\mu) = \int_{\mathbb{R}} H\left(\frac{1}{N} \sum_{i=1}^{N} \frac{1}{|B_{i,N}|} \chi_{B_{i,N}}(x) \right) \, \mathrm{d}x,$$

where $B_{i,N} = B(x_{i,N}, R_{i,N})$ with x_N satisfying $\mu = \delta_{x_N}$. Note that

$$|B_{i,N}| = C_d R_{i,N}^d = \frac{C_d}{2} \left(\min_{j \neq i} |x_{i,N} - x_{j,N}| \right)^d,$$

where $C_d = |B(0,1)|$ is the volume of the unit ball in dimension d. We clearly have $E(\rho_N) = E_N(\mu)$.

Γ-Convergence Result

- Logarithmic Entropy: Given

$$E_N(\mu) = -\frac{1}{N}\sum_{i=1}^{N}\log\left(\frac{NC_d}{2^d}\left(\min_{j\neq i}|x_{i,N}-x_{j,N}|\right)^d\right),$$

then it Γ-converges in d_2 to the logarithmic entropy $E[\mu]$.

- Nonlinear Entropy: The same holds for

$$E_N(\mu) = \int_{\mathbb{R}} \frac{1}{(m-1)N^m}\left(\sum_{i=1}^{N}\frac{1}{|B_{i,N}|}\chi_{B_{i,N}}(x)\right)^m \mathrm{d}x$$

Γ-converging to

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1. Problem & Motivation
   - Minimization of the Interaction Energy
2. Deterministic Particle Methods for Diffusions
   - Γ-Convergence
   - Numerical Scheme and Simulations
3. Deterministic Particle Methods for Aggregation-Diffusions
   - Approximation
   - The Keller-Segel Model

Discrete JKO scheme

For any N particles in $\mathbb{R}^d$, we denote their weights by $w = (w_1, \dots, w_N) \in \mathbb{R}^N$, which we assume to satisfy $\sum_{i=1}^N w_i = 1$ and $w_i \geq 0$ for all $i \in \{1, \dots, N\}$. For any such $w \in \mathbb{R}^N$, define

$$\mathcal{P}_w(\mathbb{R}^d) = \left\{ \rho \in \mathcal{P}(\mathbb{R}^d) \text{ such that } \exists x = (x_1, \dots, x_N) \in \mathbb{R}^{Nd}, \rho = \sum_{i=1}^N \frac{w_i}{|B(x_i, R_i)|} \chi_{B(x_i,R_i)} \right\},$$

where

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Note that

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Discrete Particle JKO scheme:

$$F(\tilde{\rho}) = \frac{1}{2\Delta t} d_2^2(\rho, \tilde{\rho}) + E(\tilde{\rho}), \quad \longrightarrow \quad F_N(\tilde{\rho}) = \sum_{i=1}^N w_i \frac{(x_i - \tilde{x}_i)^2}{2\Delta t} + E_N(\tilde{\rho}),$$

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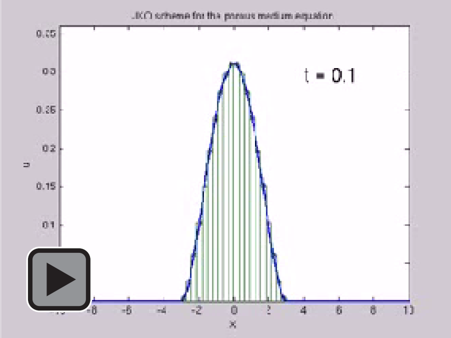
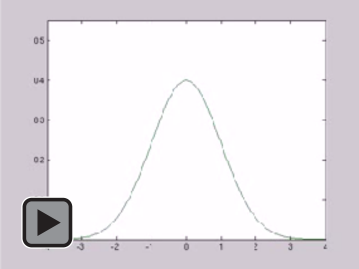
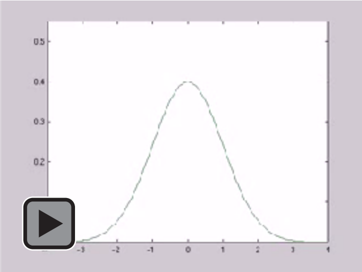
Numerical Simulation: Heat and Fokker-Planck Equations







Outline

Deterministic Particle Methods for Aggregation-Diffusions $(d = 1)$

Consider the gradient flow

$$\frac{\mathrm{d}\rho}{\mathrm{d}t}(t) = -\nabla_{\mathcal{P}_{ac,2}(\mathbb{R})} E(\rho(t)) \quad \text{on } \mathbb{R}_+.$$

$\rho \colon \mathbb{R}_+ \to \mathcal{P}_{ac,2}(\mathbb{R})$ and $\nabla_{\mathcal{P}_{ac,2}(\mathbb{R})}$ is the **2-Wasserstein gradient**:

$$\nabla_{\mathcal{P}_{ac,2}(\mathbb{R})} E(\rho) = -\nabla \cdot \left(\rho \nabla \frac{\delta E}{\delta \rho}\right) \quad \text{for any } \rho \in \mathcal{P}_{ac,2}(\mathbb{R}),$$

where $\frac{\delta E}{\delta \rho}$ is the first variation density of E at point ρ.

$E \colon \mathcal{P}_{ac,2}(\mathbb{R}) \to \overline{\mathbb{R}}$ is the **energy functional**

$$E(\rho) = \int_{\mathbb{R}} (H(\rho(x)) + U * \rho(x)) \, \mathrm{d}x \quad \text{for any } \rho \in \mathcal{P}_{ac,2}(\mathbb{R}),$$

where $H \colon [0, \infty) \to \mathbb{R}$ is the **density of internal energy** and $U \colon \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ a symmetric **interaction potential**.

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Deterministic Particle Methods for Aggregation-Diffusions

Take any $N \geq 2$ increasingly ordered particles $\{x_1, \ldots, x_N\} \subset \mathbb{R}$ with weights $\{w_i, \ldots, w_N\} \subset (0, 1)$.

The diffusion part of the energy is not defined on Dirac masses, so spread out the mass of each particle: write $B_i := B_{R_i}(x_i)$ the open ball of centre x_i and radius

$$\boxed{R_i = \frac{1}{2}\min(\Delta x_{i+1}, \Delta x_i)},$$

and define

$$\boxed{\rho_N = \sum_{i=1}^{N} \frac{w_i \chi_{B_i}}{d_i} \in \mathcal{P}_{\mathrm{ac},2}(\mathbb{R})},$$

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Deterministic Particle Methods for Aggregation-Diffusions

Assume $H(0) = 0$ and compute

$$\int_{\mathbb{R}} H(\rho_N(x))\,\mathrm{d}x = \int_{\mathbb{R}} H\left(\frac{1}{N}\sum_{i=1}^{N}\frac{\chi_{B_i}(x)}{|B_i|}\right)\mathrm{d}x = \sum_{i=1}^{N} d_i H\left(\frac{w_i}{d_i}\right).$$

Define now the **discrete energy** $E_N : \mathbb{R}^N \to \overline{\mathbb{R}}$ by

$$E_N(x) = \sum_{i=1}^{N} d_i H\left(\frac{w_i}{d_i}\right) + \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} w_i w_j U(x_i - x_j), \quad x \in \mathbb{R}^N.$$

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Deterministic Particle Methods for Aggregation-Diffusions

We define a discrete gradient flow:

$$w\frac{\mathrm{d}x}{\mathrm{d}t}(t) \in -\partial E_N(x(t)) \quad \text{for all } t \in \mathbb{R}_+,$$

where $w\frac{\mathrm{d}x}{\mathrm{d}t}$ is the vector $(w_1 x_1, \ldots, w_N x_N) \in \mathbb{R}^N$ if we write $x := (x_1, \ldots, x_N)$, and ∂ stands for the subdifferential.

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Remark. The gradient flow has here the structure of a **differential inclusion** since the discrete energy E_N has no well-defined gradient because of the presence of the minimum function (in d_i).

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Deterministic Particle Methods for Aggregation-Diffusions

Definition (p-approximation of minimum function). Let us define, for any $p > 0$, the function $\min_p \colon [0,\infty)^2 \to [0,\infty)$ as

$$\min_p(x,y) = \begin{cases} \left(\dfrac{x^{-p}+y^{-p}}{2}\right)^{-1/p} & \text{for all } x,y \in (0,\infty) \\ 0 & \text{otherwise} \end{cases}.$$

We define the ***p*-approximated discrete energy** by

$$E_{N,p} = \sum_{i=1}^{N} w_i \log \frac{w_i}{d_{i,p}} + \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} w_i w_j U(x_i - x_j),$$

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Deterministic Particle Methods for Aggregation-Diffusions

The p-approximated discrete energy $E_{N,p}$ has a well-defined gradient.

The p-approximated gradient flows writes then as the ODE system

$$w_i \frac{\mathrm{d}x_i}{\mathrm{d}t}(t) = -\nabla_{x_i} E_{N,p}(x_1(t), \dots, x_N(t)) \quad \text{for all } t \in \mathbb{R}_+.$$

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For the heat equation ($H(x) = x \log x$ and $W = 0$) we are able to show that the p-approximated gradient flow converges to the continuum gradient flow in the Serfaty sense.[1]

To find the solution to the p-approximated ODE system we use an explicit version of the following JKO scheme:

$$x^{n+1} := \operatorname*{argmin}_{x \in \mathbb{R}^N} \left(\sum_{i=1}^{N} w_i \frac{(x_i^n - x_i)^2}{2\Delta t} + E_{N,p}(x) \right).$$

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Outline

Deterministic Particle Methods for Aggregation-Diffusions

The Keller-Segel equation ($H(x) = x \log x$ and $W(x) = 2\chi \log |x|$).

$$\frac{\partial \rho}{\partial t} = \Delta \rho + 2\chi \nabla \cdot (\rho \nabla \log |\cdot| * \rho) \quad \text{on } \mathbb{R}_+ \times \mathbb{R},$$

where χ is an **interaction parameter** quantifying the "strength" of the attraction.

Write $M_2(t) := \int_{\mathbb{R}} |x|^2 \, d\rho(t,x)$. Theoretically, it is easy to check that

$$\frac{dM_2}{dt}(t) = 2(1-\chi) \quad \text{for all } t \in [0,\infty).$$

Thus we have three cases:

Subcritical. $\chi < 1$: solutions exist for all times; the diffusion wins over the attraction.

Critical. $\chi = 1$.

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Deterministic Particle Methods for Aggregation-Diffusions

Write $M_2^{N,p}(t) := \int_{\mathbb{R}} |x|^2 \, \mathrm{d}\rho_{N,p}(t,x)$, where $\rho_{N,p} = \sum_{i=1}^{N} \frac{w_i \chi_{B_i}}{d_{i,p}}$. Interestingly, using our p-approximated discrete gradient flow, we can compute

$$\frac{\mathrm{d}M_2^{N,p}}{\mathrm{d}t}(t) = 2(1-\chi) + \underset{\substack{N\to\infty \\ p\to\infty}}{\mathcal{O}}(1) \quad \text{for all } t \in [0,\infty).$$

Adaptive time step. To catch blow-up we implement the following adaptive time step method.

1. Initialize $\Delta t = 10^{-5}$ and fix $\varepsilon < 1$.
2. If $\Delta t > \frac{\varepsilon d_{i,p}}{2\left|\frac{\mathrm{d}x_i}{\mathrm{d}t}\right|}$, then define $\Delta t_i := \frac{\varepsilon d_{i,p}}{2\left|\frac{\mathrm{d}x_i}{\mathrm{d}t}\right|}$.
3. Let I be the set of indices for which the if-loop above was entered. If $I = \emptyset$, then choose $\Delta t = \Delta t$. If $I \neq \emptyset$, then choose $\Delta t = \min_{i\in I} \Delta_i$.
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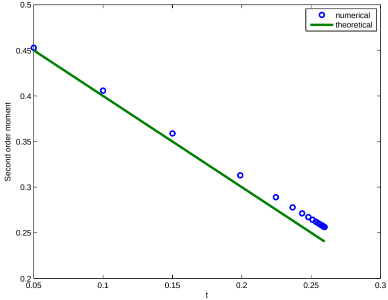


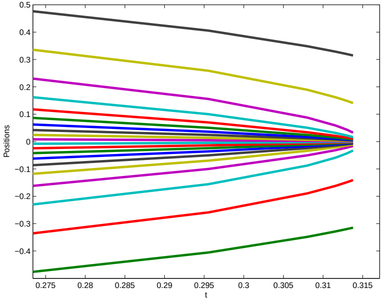
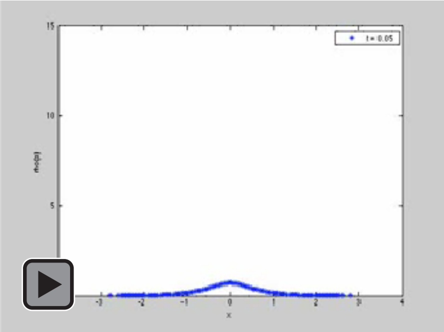
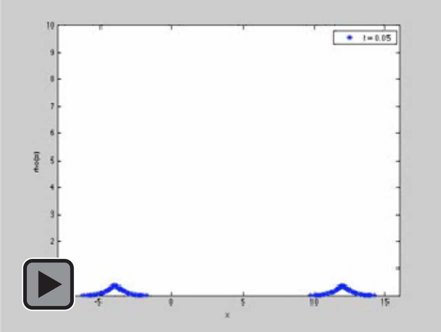


Figure : Evolution of second order moment with $\chi = 1.5$ and $N = 100$ (left). Evolution of positions before numerical blow-up with $\chi = 1.5$ and $N = 50$ (right).

Deterministic Particle Methods for Aggregation-Diffusions





Videos.
Keller Segel – $\chi = 1.5$; $N = 100$; one Gaussian
Keller Segel – $\chi = 3$; $N = 100$; two Gaussians