Gradient Flows: Qualitative Properties & Numerical Schemes

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Imperial College London

RICAM, December 2014

Outline

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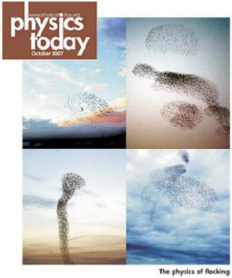
Swarming by Nature or by design?



Fish schools and Birds flocks.

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 ...), fishes, birds, micro-organisms (myxo-bacteria, ...) 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.
- Attraction Region: A_k.
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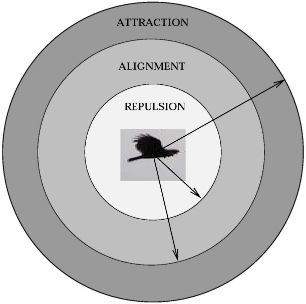

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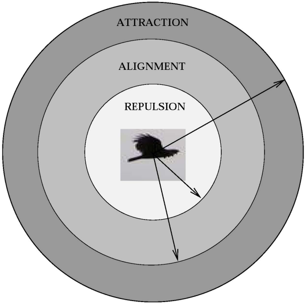

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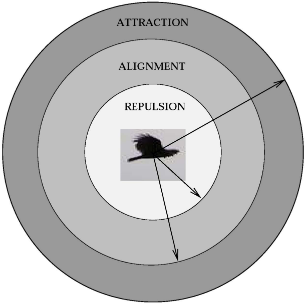
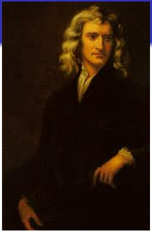


2nd Order Model: Newton's like equations



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

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

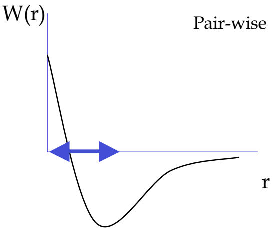
Model assumptions:

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

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

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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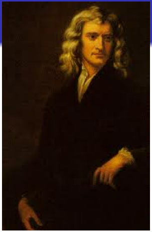

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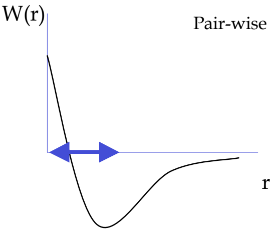

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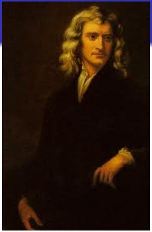

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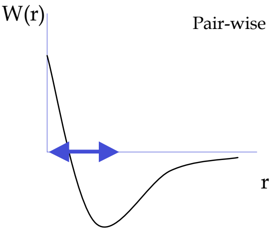

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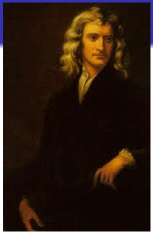

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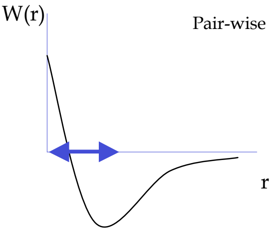
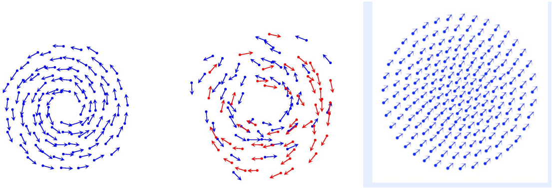


Model with an asymptotic speed

Typical patterns: milling, double milling or flocking:



1st Order Friction Model:

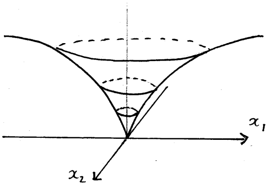
Edelshtein-Keshet, Mogilner (JMB 2000): Assume the variations of the velocity and speed are much smaller than spatial variations, then from Newton's equation:

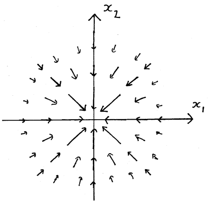
$$m\frac{d^2x_i}{d^2t} + \alpha\frac{dx_i}{dt} + \sum_{j\neq i}\nabla W(|x_i - x_j|) = 0$$

so finally, we obtain

$$\frac{dx_i}{dt} = -\sum_{j\neq i}\nabla W(|x_i - x_j|) \qquad \text{in the continuum setting} \Rightarrow \qquad \begin{cases} \frac{\partial\rho}{\partial t} + \operatorname{div}(\rho v) = 0 \\ v = -\nabla W * \rho \end{cases}$$

Purely Aggregative Case: $W : \mathbb{R}^d \longrightarrow \mathbb{R}$





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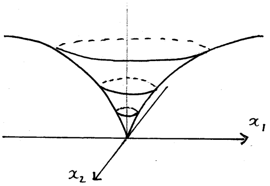

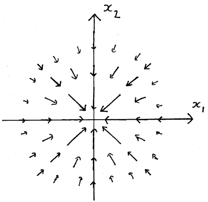

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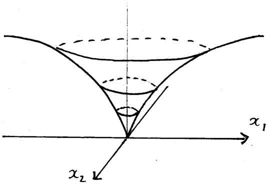

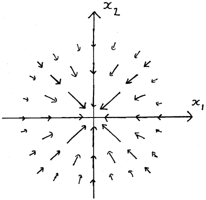

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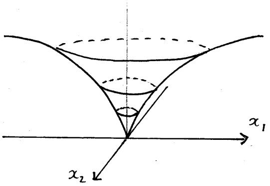

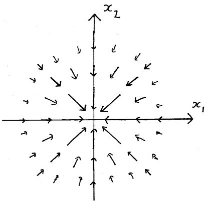

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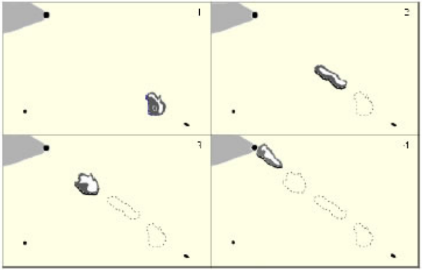
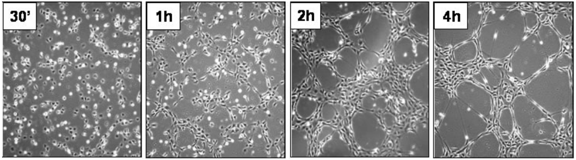
Chemotaxis





Cell movement and aggregation by chemical interaction.

KS System

Keller-Segel System:

Cells positions are assumed to fluctuate, in the sense of a Brownian motion, around the dominated trend to follow the trail of the largest concentration of chemoattractant:

$$x' = \nabla c(x,t) + \Gamma(t).$$

where $\Gamma(t)$ is a Wiener process with fixed variance. The chemoattractant diffuses spatially and is produced by the cells themselves.

$$\begin{cases} \dfrac{\partial n}{\partial t}(x,t) = \Delta n(x,t) - \chi \nabla \cdot (n(x,t) \nabla c(x,t)) & x \in \mathbb{R}^2,\ t > 0, \\ \dfrac{\partial c}{\partial t}(x,t) - \Delta c(x,t) = n(x,t) - \alpha c(x,t) & x \in \mathbb{R}^2,\ t > 0, \\ n(x, t = 0) = n_0 \geq 0 & x \in \mathbb{R}^2. \end{cases}$$

Patlak (1953), Keller-Segel (1971), Nanjundiah (1973).

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Huge Literature: Horstmann reviews (2003& 2004), Perthame review (2004).

Smoluchowski-Poisson in gravitational collapse literature.

Conservations:

- Conservation of mass:

$$M := \int_{\mathbb{R}^2} n_0(x)\, dx = \int_{\mathbb{R}^2} n(x,t)\, dx$$

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Second Moment

Distributional Solution:

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$$\frac{d}{dt}\int_{\mathbb{R}^2} \psi(x)\, n(x,t)\, dx =$$

$$\int_{\mathbb{R}^2} \Delta\psi(x)\, n(x,t)\, dx - \frac{\chi}{4\pi}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} [\nabla\psi(x) - \nabla\psi(y)] \cdot \frac{x-y}{|x-y|^2}\, n(x,t)\, n(y,t)\, dx\, dy$$

holds in the distributional sense in $(0,T)$ and $n(0) = n_0$.

Evolution of second moment:

$$\frac{d}{dt}\int_{\mathbb{R}^2} |x|^2\, n(x,t)\, dx = 4M - \frac{\chi}{2\pi} M^2,$$

Struggle between diffusion and aggregation. Balance between these two mechanisms happens precisely at the critical mass $\chi M = 8\pi$.

Fix $M = 1$ and $M_1 = 0$ without loss of generality.

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Distributional Solution:

We shall say that $n \in C^0\big([0,T); L^1_{\text{weak}}(\mathbb{R}^2)\big)$ is a weak solution to the PKS system if for all test functions $\psi \in \mathcal{D}(\mathbb{R}^2)$,

$$\frac{d}{dt}\int_{\mathbb{R}^2} \psi(x)\, n(x,t)\, dx =$$

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holds in the distributional sense in $(0,T)$ and $n(0) = n_0$.

Evolution of second moment:

$$\frac{d}{dt}\int_{\mathbb{R}^2} |x|^2\, n(x,t)\, dx = 4M - \frac{\chi}{2\pi}M^2,$$

Struggle between diffusion and aggregation. Balance between these two mechanisms happens precisely at the critical mass $\chi M = 8\pi$.

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Cases

PKS Cases:

- **Subcritical Case, $\chi < 8\pi$:** Jägger-Luckhaus (1992) without optimal critical mass. Dolbeault-Perthame (2004), Blanchet-Dolbeault-Perthame (2006) proved global existence of free-energy solutions.
- **Supercritical Case, $\chi > 8\pi$:** Herrero-Xelazquez (1996) particular solutions blow up in finite time. Xelazquez (2002-2004) proves formal asymptotic expansions for the behavior after blow-up. Dolbeault-Schmeiser (2007) have introduced a concept of solution due to Poupaud for dealing with solutions after blow-up.
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Rescaled System

Let us define the rescaled functions ρ and v by:

$$n(t,x) = \frac{1}{R^d(t)}\,\rho\left(\tau(t), \frac{x}{R(t)}\right) \quad \text{and} \quad c(x,t) = v\left(\tau(t), \frac{x}{R(t)}\right)$$

with

$$R(t) = \sqrt{1+2t} \quad \text{and} \quad \tau(t) = \log R(t)\,.$$

The rescaled system with $\rho(0,x) = \rho^0 = n_0 \geq 0$ is

$$\begin{cases} \dfrac{\partial \rho}{\partial t}(t,x) = \Delta\rho(t,x) + \nabla\cdot\{\rho(t,x)\,[x - \chi\nabla v(t,x)]\} & t > 0\,,\ x \in \mathbb{R}^d\,, \\ v(t,x) = -\dfrac{1}{d\,\pi}\,\log|\cdot| * \rho(t,x) & t > 0\,,\ x \in \mathbb{R}^d\,. \end{cases}$$

In the rescaled variables, the free energy becomes

$$\mathcal{G}[\rho] = \int_{\mathbb{R}^d} \rho(x)\log\rho(x)\,dx + \frac{1}{2}\int_{\mathbb{R}^d} |x|^2\rho(x)\,dx + \frac{\chi}{2\,d\,\pi}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \log|x-y|\,\rho(x)\,\rho(y)\,dx\,dy$$

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Nonlinear diffusion PKS system

Xolume effects can be taken into account by considering nonlinear diffusion (Calvez& C., JMPA 2006) as:

$$\begin{cases} \dfrac{\partial \rho}{\partial t}(t,x) & = \operatorname{div}\left[\nabla \rho^m(t,x) - \rho(t,x)\nabla c(t,x)\right] \qquad t>0\,,\ x\in\mathbb{R}^d\,, \\ -\Delta c(t,x) & = \rho(t,x)\,, \qquad t>0\,,\ x\in\mathbb{R}^d\,, \end{cases}$$

Free Energy:

The corresponding free energy is

$$\mathcal{F}_m[\rho](t) := \int_{\mathbb{R}^d} \frac{\rho^m}{m-1}\,dx - \frac{c_d}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \frac{1}{|x-y|^{d-2}}\,\rho(t,x)\,\rho(t,y)\,dx\,dy$$

with $c_d^{-1} := (d-2)2\,\pi^{d/2}/\Gamma(d/2)$.

Diffusion to compensate exactly drift by scaling (Blanchet, C. & Laurençot, CXPDE 2008) is

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Outline

General Entropy Functional[1]

$$\mathcal{F}[\rho] = \mathcal{U}[\rho] + \mathcal{X}[\rho] + \mathcal{W}[\rho]$$

with

$$\mathcal{U}[\rho] = \int_{\mathbb{R}^d} U(\rho(x))\, dx \quad \text{internal energy}$$

$$\mathcal{X}[\rho] = \int_{\mathbb{R}^d} X(x)\rho(x)\, dx \quad \text{confinement energy}$$

$$\mathcal{W}[\rho] = \frac{1}{2}\int_{\mathbb{R}^{2d}} W(x-y)\rho(x)\rho(y)\, dx\, dy \quad \text{interaction energy}$$

Let us write the formal gradient flow equation as before:

$$\frac{\partial \rho}{\partial t} = \operatorname{div}\left(\rho \nabla \frac{\delta \mathcal{F}}{\delta \rho}\right), \qquad (x \in \mathbb{R}^d, t > 0).$$

and the dissipation of entropy is defined as

$$\frac{d}{dt}\mathcal{F}[\rho] = -D[\rho] \quad \text{with} \quad D[\rho] = \int_{\mathbb{R}^d} |\xi|^2 \rho(x)\, dx,$$

with

$$\xi = \nabla\left[U'[\rho] + X + W * \rho\right] = \nabla \frac{\delta \mathcal{F}}{\delta \rho}.$$

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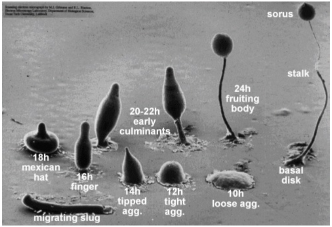
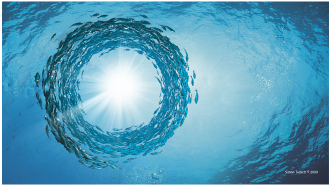
Nonlinear continuity equations

Included models:

- $U(s) = s \log s$, $X = 0$, $W = 0$ heat equation.
- $U(s) = \frac{1}{m-1} s^m$, $X = W = 0$ porous medium ($m > 1$) or fast diffusion ($0 < m < 1$).
- $U(s) = s \log s$, X given, $W = 0$, Fokker Planck equations.
- $U(s) = s \log s$, $X = 0$, $W = \log(|x|)$, Patlak-Keller-Segel model.
- $U = 0$, $X = 0$, $W = \frac{1}{a}|x|^a - \frac{1}{b}|x|^b$ correspond to attraction-(repulsion) potentials in swarming, herding and aggregation models.



(a) Dictyostelium discoideum



(b) Fish school

Outline

Definition of the distance[2]

Transporting measures:

Given $T : \mathbb{R}^d \longrightarrow \mathbb{R}^d$ mesurable, we say that $\nu = T\#\mu$, if $\nu[K] := \mu[T^{-1}(K)]$ for all mesurable sets $K \subset \mathbb{R}^d$, equivalently

$$\int_{\mathbb{R}^d} \varphi \, d\nu = \int_{\mathbb{R}^d} (\varphi \circ T) \, d\mu$$

for all $\varphi \in C_o(\mathbb{R}^d)$.

Random variables:

Say that X is a random variable with law given by μ, is to say $X : (\Omega, \mathcal{A}, P) \longrightarrow (\mathbb{R}^d, \mathcal{B}_d)$ is a mesurable map such that $X\#P = \mu$, i.e.,

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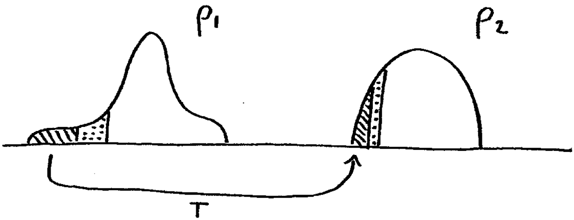
Two piles of sand!

Energy needed to transport m kg of sand from $x = a$ to $x = b$:

$$\text{energy} = m|a - b|^2$$



$d_2^2(\rho_1, \rho_2)$ = Among all possible ways to transport the mass from ρ_1 to ρ_2, find the one that minimizes the total energy

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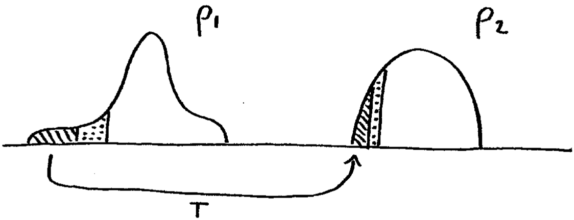

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Kantorovich-Rubinstein-Wasserstein Distance $p = 1, 2$:

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where the transference plan π runs over the set of joint probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals μ and $\nu \in \mathcal{P}_p(\mathbb{R}^d)$ and (X,Y) are all possible couples of random variables with μ and ν as respective laws.

Monge's optimal mass transport problem:

Find

$$I := \inf_T \left\{ \int_{\mathbb{R}^d} |x - T(x)|^p \, d\mu(x);\ \nu = T\#\mu \right\}^{1/p}.$$

Take $\gamma_T = (1_{\mathbb{R}^d} \times T)\#\mu$ as transference plan π.

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where the transference plan π runs over the set of joint probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals μ and $\nu \in \mathcal{P}_p(\mathbb{R}^d)$ and (X,Y) are all possible couples of random variables with μ and ν as respective laws.

Monge's optimal mass transport problem:

Find

$$I := \inf_T \left\{ \int_{\mathbb{R}^d} |x - T(x)|^p \, d\mu(x);\ \nu = T\#\mu \right\}^{1/p}.$$

Take $\gamma_T = (1_{\mathbb{R}^d} \times T)\#\mu$ as transference plan π.

Definition of the distance

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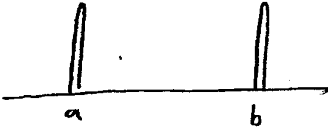
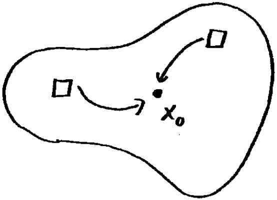
Three examples



$$d_2^2(\delta_a, \delta_b) = |a - b|^2$$



$$d_2^2(\rho, \delta_{X_0}) = \int |X_0 - y|^2 d\rho(y)$$
$$= \mathrm{Xar}\ (\rho)$$

Outline

Euclidean Wasserstein Distance

Convergence Properties

1. **Convergence of measures:** $d_2(\mu_n, \mu) \to 0$ is equivalent to $\mu_n \rightharpoonup \mu$ weakly-* as measures and convergence of second moments.
2. **Weak lower semicontinuity:** Given $\mu_n \rightharpoonup \mu$ and $\nu_n \rightharpoonup \nu$ weakly-* as measures, then
$$d_2(\mu, \nu) \leq \liminf_{n\to\infty} d_2(\mu_n, \nu_n).$$
3. **Completeness:** The space $\mathcal{P}_2(\mathbb{R}^d)$ endowed with the distance d_2 is a complete metric space.

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One dimensional Case

Distribution functions:

In one dimension, denoting by $F(x)$ the distribution function of μ,

$$F(x) = \int_{-\infty}^{x} d\mu,$$

we can define its pseudo inverse:

$$F^{-1}(\eta) = \inf\{x : F(x) > \eta\} \qquad \text{for } \eta \in (0,1),$$

we have $F^{-1} : ((0,1), \mathcal{B}_1), d\eta) \longrightarrow (\mathbb{R}, \mathcal{B}_1)$ is a random variable with law μ, i.e., $F^{-1}\#d\eta = \mu$

$$\int_{\mathbb{R}} \varphi(x)\, d\mu = \int_0^1 \varphi(F^{-1}(\eta))\, d\eta = \mathbb{E}\left[\varphi(X)\right].$$

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Wasserstein distance:

In one dimension, it can be checked[a] that given two measures μ and ν with distribution functions $F(x)$ and $G(y)$ then, $(F^{-1} \times G^{-1})\#d\eta$ has joint distribution function $H(x,y) = \min(F(x), G(y))$. Therefore, in one dimension, the optimal plan is given by $\pi_{opt}(x,y) = (F^{-1} \times G^{-1})\#d\eta$, and thus

$$d_p(\mu,\nu) = \left(\int_0^1 [F^{-1}(\eta) - G^{-1}(\eta)]^p \, d\eta \right)^{1/p} = \|F^{-1} - G^{-1}\|_{L^p(\mathbb{R})}$$

$1 \leq p < \infty$.

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Outline

Nonlinear continuity equations

Let us consider a time dependent unknown probability density $\rho(t,\cdot)$ on a domain $\Omega \subset \mathbb{R}^d$, which satisfies the nonlinear continuity equation

$$\partial_t \rho = -\nabla \cdot (\rho u) := \nabla \cdot \left(\rho \nabla \left[U'(\rho) + X + W * \rho\right]\right).$$

- $U : \mathbb{R}^+ \to \mathbb{R}$ denotes the internal energy.
- $X : \mathbb{R}^d \to \mathbb{R}$ is the confining potential.
- $W : \mathbb{R}^d \to \mathbb{R}$ corresponds to an interaction potential.

Nonlinear velocity is given by $u = -\nabla \frac{\delta \mathcal{F}}{\delta \rho}$, where $\mathcal{F}$ denotes the free energy or entropy functional

$$\mathcal{F}(\rho) = \int_{\mathbb{R}^d} U(\rho)dx + \int_{\mathbb{R}^d} X(x)\rho(x)dx + \frac{1}{2}\int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y)\rho(x)\rho(y)dxdy.$$

Free energy is decreasing along trajectories

$$\frac{d}{dt}\mathcal{F}(\rho)(t) = -\int_{\mathbb{R}^d} \rho(x,t)|u(x,t)|^2 dx.$$

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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

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

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- Solutions ρ can be constructed by the following variational scheme:

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with $\mathcal{K} = \{\rho \in L^1_+(\mathbb{R}^d) : \int_{\mathbb{R}^d} \rho(x)dx = M, |x|^2\rho \in L^1(\mathbb{R}^d)\}$.

- Xariational scheme corresponds to the time discretization of an abstract gradient flow in the space of probability measures.
- Solutions can be constructed by this variational scheme; naturally preserve positivity and the free-energy decreasing property.
- Under general assumptions on smooth potentials W and X and internal energy U together with λ-convexity, this scheme is shown to be convergent, see AGS book.

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Outline

Log HLS Inequality by Carlen& Loss

Let f be a non-negative function in $L^1(\mathbb{R}^d)$ such that $f\log f$ and $f\log(1+|x|^2)$ belong to $L^1(\mathbb{R}^d)$. If

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then

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with $C(d) := (1/2)\log\pi + (1/d)\log[\Gamma(d/2)/\Gamma(d)] + (1/2)[\psi(d)-\psi(d/2)]$ where ψ is the logarithmic derivative of the Γ-function.

Equality cases:

The equality is only achieved by

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Rescaled System

$M = 1$ and general dimension in this part keeping the convolution.

Let us define the rescaled functions ρ and v by:

$$n(t,x) = \frac{1}{R^d(t)}\,\rho\left(\tau(t), \frac{x}{R(t)}\right) \quad \text{and} \quad c(x,t) = v\left(\tau(t), \frac{x}{R(t)}\right)$$

with

$$R(t) = \sqrt{1+2t} \quad \text{and} \quad \tau(t) = \log R(t)\,.$$

The rescaled system with $\rho(0,x) = \rho^0 = n_0 \geq 0$ is

$$\begin{cases} \dfrac{\partial \rho}{\partial t}(t,x) = \Delta \rho(t,x) + \nabla \cdot \{\rho(t,x)\,[x - \chi \nabla v(t,x)]\} & t > 0\,,\ x \in \mathbb{R}^d\,, \\ v(t,x) = -\dfrac{1}{d\,\pi}\,\log|\cdot| * \rho(t,x) & t > 0\,,\ x \in \mathbb{R}^d\,. \end{cases}$$

In the rescaled variables, the free energy becomes

$$\mathcal{G}[\rho] = \int_{\mathbb{R}^d} \rho(x)\log\rho(x)\,dx + \frac{1}{2}\int_{\mathbb{R}^d} |x|^2\rho(x)\,dx + \frac{\chi}{2\,d\,\pi}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \log|x-y|\,\rho(x)\,\rho(y)\,dx\,dy$$

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$$\mathcal{G}[\rho] = \int_{\mathbb{R}^d} \rho(x)\log\rho(x)\,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^d} |x|^2\rho(x)\,\mathrm{d}x + \frac{\chi}{2\,d\,\pi}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \log|x-y|\,\rho(x)\,\rho(y)\,\mathrm{d}x\,\mathrm{d}y$$

Estimates from below

A priori estimates

The functional $\mathcal{G}$ is bounded from below on the set

$$\mathcal{K} := \left\{ \rho \in L^1_+(\mathbb{R}^d) : \int_{\mathbb{R}^d} \rho(t,x) = 1,\ |x|^2 \rho \in L^1(\mathbb{R}^d),\ \int_{\mathbb{R}^d} \rho(t,x) |\log \rho(t,x)| \, \mathrm{d}x < \infty \right\}$$

if and only if $\chi \le \chi_c := 2\, d^2 \pi$. In addition, if $\chi < \chi_c$ we have on every subset $\{\mathcal{G} \le C\}$,

i) *no concentration:* $\displaystyle\int_{\mathbb{R}^d} \rho |\log \rho| \le C$,

ii) *mass confinement:* $\displaystyle\int_{\mathbb{R}^d} |x|^2 \rho \le C$,

As a consequence, every level subset $\{\mathcal{G} \le C\}$ is equi-integrable.

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Estimates from below: Proof

Step 1.- Rewrite

$$\mathcal{G}[\rho](t) = (1-\theta)\int_{\mathbb{R}^d} \rho(t,x)\log\rho(t,x)\,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^d} |x|^2\rho(t,x)\,\mathrm{d}x$$

$$+\,\theta d\left[\frac{1}{d}\int_{\mathbb{R}^d}\rho(t,x)\log\rho(t,x)\,\mathrm{d}x + \frac{\chi}{2\,d^2\,\pi\,\theta}\iint_{\mathbb{R}^d\times\mathbb{R}^d}\rho(t,x)\,\rho(t,y)\,\log|x-y|\,\mathrm{d}x\,\mathrm{d}y\right].$$

Log HLS inequality controls the third term if we choose $\theta = \chi/\chi_c$.

Step 2.- For any probability density $u \in L^1_+(\mathbb{R}^d)$ with finite second moment and entropy, $u\log u$ is uniformly bounded in $L^1(\mathbb{R}^d)$ and we have

$$\int_{\mathbb{R}^d} u(x)\,|\log u(x)|\,\mathrm{d}x \le \int_{\mathbb{R}^d} u(x)\left(\log u(x) + \frac{1}{2}|x|^2\right)\mathrm{d}x + d\log(4\pi) + \frac{2}{e}\,.$$

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Estimates from below: Proof

Step 3.- We finish the proof for the subcritical case in which $\theta < 1$ since

$$\mathcal{G}[\rho](t) \geq (1-\theta) \int_{\mathbb{R}^d} \rho(t,x) \, |\log \rho(t,x)| \, \mathrm{d}x + \frac{\theta}{2} \int_{\mathbb{R}^d} |x|^2 \rho(t,x) \, \mathrm{d}x + C.$$

Step 4.- Scaling $\rho_\lambda(x) = \lambda^d \rho(\lambda x)$

$$\mathcal{G}[\rho_\lambda] = \mathcal{G}[\rho] + d\left(1 - \frac{\chi}{\chi_c}\right) \log \lambda + \frac{\lambda^{-2} - 1}{2} \int_{\mathbb{R}^d} |x|^2 \rho \, \mathrm{d}x \, .$$

$\lambda \mapsto \mathcal{G}[\rho_\lambda]$ is clearly not bounded from below if $\chi > \chi_c$.

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Outline

Existence of minimizers

We consider a time-step $\tau > 0$, an initial datum $\rho^0 \in \mathcal{P}_2^{ac}(\mathbb{R}^d)$. We introduce the sequence $(\rho_\tau^n)_{n\in\mathbb{N}}$ recursively defined by $\rho_\tau^0 = \rho^0$ and

$$\rho_\tau^{n+1} \in \arg\inf_{\rho\in\mathcal{K}} \left\{ \mathcal{G}[\rho] + \frac{1}{2\tau} d_2^2(\rho_\tau^n, \rho) \right\} .$$

Existence of minimizers:

Let ρ_0 satisfies

$$(1 + |x|^2)\, n_0 \in L_+^1(\mathbb{R}^d) \quad \text{and} \quad n_0 \log n_0 \in L^1(\mathbb{R}^d) .$$

and $\chi < \chi_c$, then there recursively exists a minimizer to the previous problem.

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Convergence Theorem

Theorem

Under assumptions

$$(1 + |x|^2)\, n_0 \in L^1_+(\mathbb{R}^d) \quad \textit{and} \quad n_0 \log n_0 \in L^1(\mathbb{R}^d)\ ,$$

let us construct the family $(\rho_\tau)_{\tau>0}$ *as*

$$\rho_\tau(t) = \left(\frac{(n+1)\tau - t}{\tau} \mathrm{Id} + \frac{t - n\tau}{\tau} \nabla \varphi^n \right) \# \rho^n_\tau$$

with $\nabla\varphi^n$ *being the optimal map transporting* ρ^n_τ *onto* ρ^{n+1}_τ*, for any* $t \in [n\tau, (n+1)\tau)$.

If $\chi < \chi_c$*, then the family* $(\rho_\tau)_{\tau>0}$ *admits a sub-sequence converging weakly in* $C^0([0,T], L^1_{\mathrm{weak}}(\mathbb{R}^d))$ *to a distributional solution of the PKS system.*

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Outline

Brief Remainder

In the case of the real line, consider μ and ν two absolutely continuous measures with respect to the Lebesgue measure, of respective densities f and g, and of cumulative distribution functions F and G. As the cumulative distribution function is non-decreasing we can define the pseudo-inverse function by

$$X(z) = F^{-1}(z) := \inf\{x : F(x) \geq z\} .$$

The transport map is $\varphi' = F^{-1} \circ G$ and the Wasserstein distance can be expressed in the following more tractable way

$$d_2^2(\mu, \nu) = \int_0^1 |F^{-1}(w) - G^{-1}(w)|^2 \, dw .$$

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Implicit Euler Scheme

Let F_n and F_{n+1} be the cumulative distribution functions associated respectively to ρ_τ^n and ρ_τ^{n+1}.

By the expression of the Wasserstein distance on the real line, the JKO scheme can be rewritten in terms of $X_n = F_n^{-1}$ and $X_{n+1} = F_{n+1}^{-1}$ as the gradient flow of the inverse distribution function subject to L^2–metric structure:

$$X_{n+1} = \inf_W \left[\mathcal{G}[W] + \frac{1}{2\tau} \|W - X_n\|^2_{L^2(0,1)} \right] .$$

The Euler-Lagrange equation is

$$-\frac{X_{n+1}(w) - X_n(w)}{\tau} = \frac{\partial}{\partial w}\left[\left(\frac{\partial X_{n+1}(w)}{\partial w}\right)^{-1}\right] + X_{n+1}(w) + \frac{\chi}{\pi} H[X_{n+1}]$$

where H corresponds to the Hilbert transform defined by

$$H[X](w) := \frac{1}{\pi} \lim_{\varepsilon \to 0} \int_{|X(w)-X(z)| \geq \varepsilon} \frac{1}{X(w) - X(z)} \, dz .$$

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Theorem on Fully Discrete Scheme

If we set $X_n^i := X_n(ih)$, for any $i = 0 \cdots N$, and $Nh = 1$, the finite difference discretisation in space is the following implicit Euler scheme in rescaled variables,

$$-\frac{X_{n+1}^i - X_n^i}{\tau} = \frac{1}{X_{n+1}^{i+1} - X_{n+1}^i} - \frac{1}{X_{n+1}^i - X_{n+1}^{i-1}} + X_{n+1}^i + \frac{\chi}{\pi} \sum_{j \neq i} \frac{1}{X_{n+1}^i - X_{n+1}^j} .$$

with initial condition X_0 associated to ρ_0.

We impose Neumann boundary conditions in the X-problem, so that the 'centre of mass' is conserved:

$$\forall n \ \sum_{i=0}^{N} X_n^i = 0.$$

Theorem

Assume $\chi(1-h) < \chi_c$. Then the solution of the numerical scheme converges to a unique steady-state of the problem with exponential rate.

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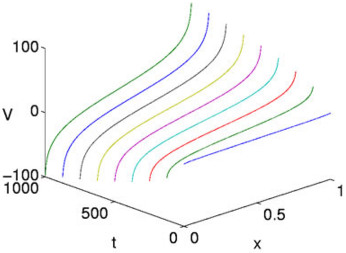
Outline

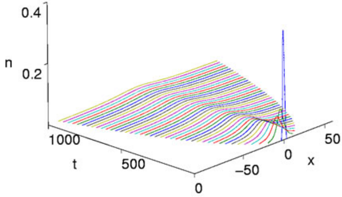
Not rescaled: $\chi = \pi$

Initial data:

Starting with the centered compactly supported initial data,

$$X_0^i = 2\,\frac{w_i - 0.5}{\left[(w_i + 0.01)\,(1.01 - w_i)\right]^{1/4}}\,,$$





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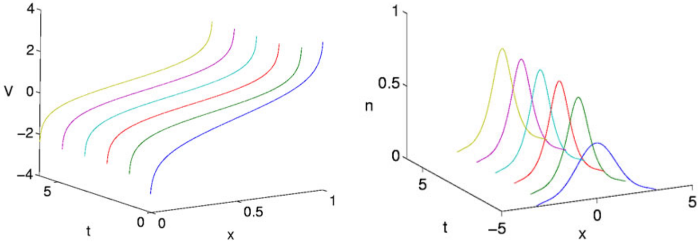
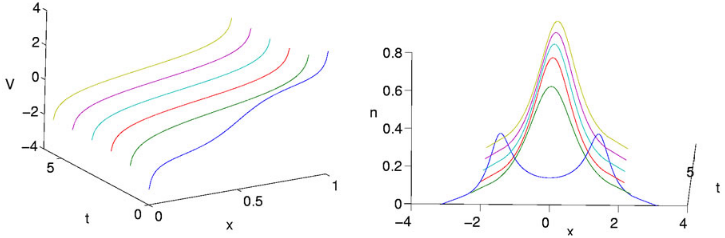


Rescaled variables: $\chi = \pi$

Two peaks initial data:

Starting with the centered compactly supported initial data,

$$X_0^i = \frac{\exp\left[10\,(w_i - 0.5)\right] - 1}{\left[(w_i + 0.01)\,(1.01 - w_i)\right]^{1/4}}\,,$$



Not rescaled: $\chi = (5/2)\,\pi$

Initial data:

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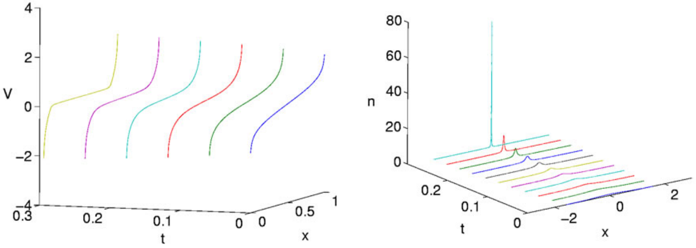
$$X_0^i = 2\,\frac{w_i - 0.5}{\left[(w_i + 0.01)\,(1.01 - w_i)\right]^{1/4}}\,,$$

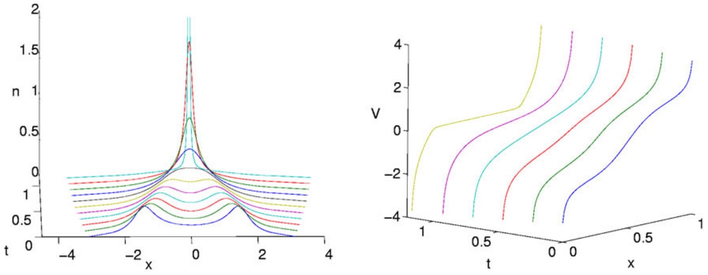


Not rescaled: $\chi = 3\pi$

Two symmetric peaks:

Starting with the centered compactly supported initial data,

$$X_0^i = \frac{\exp\left[10\,(w_i - 0.5)\right] - 1}{\left[(w_i + 0.01)\,(1.01 - w_i)\right]^{1/4}} \,,$$

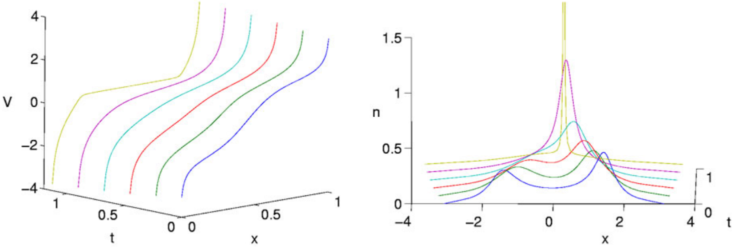


Not rescaled: $\chi = 3\pi$

Two asymmetric peaks:

Starting with the centered compactly supported initial data,

$$X_0^i = \frac{\exp\left[10\,(w_i - 0.45)\right] - 1}{\left[(w_i + 0.01)\,(1.01 - w_i)\right]^{1/4}},$$



Not rescaled: $\chi = 5\pi$

Two symmetric peaks:

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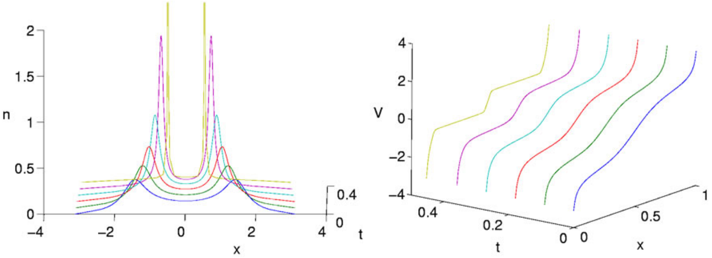

Conclusions

- The gradient flow interpretation induces a natural lagrangian or particle method on a grid or moving mesh method.
- It is a good solution to track accurately blow-up time and profiles for variant of KS in 1D.
- References:
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