



Mathematical
Institute

Aggregation–Diffusion Equations: concentration vs simplification

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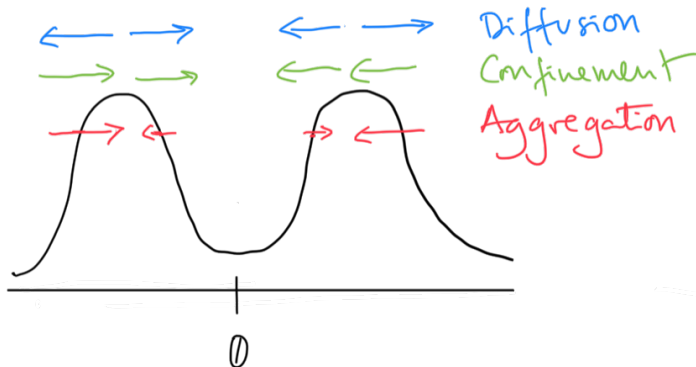
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The aim of this talk is to explain the modeling and theory behind the following model for aggregation-diffusion phenomena:

$$\frac{\partial \rho}{\partial t} = \operatorname{div} \left(\underbrace{\rho \nabla (U'(\rho))}_{\text{Diffusion}} + \underbrace{V}_{\text{Confinement}} + \underbrace{W * \rho}_{\text{Aggregation}} \right) \quad (\text{ADE})$$

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We will discuss the range of power-type aggregation and diffusion

$$U'(\rho) = \frac{m}{m-1} \rho^{m-1}, \quad V(x) = \frac{|x|^\alpha}{\alpha}, \quad \text{and} \quad W(x) = \frac{|x|^\lambda}{\lambda}.$$

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If V, W are bounded below, we can always assume $V, W \geq 0$.

Modelling

Classical results of asymptotics

Calculus of Variations approach

- Gradient flows

- Free-energy minimisation for ADE

A tale of two examples (back to PDE theory)

- An example of asymptotic concentration

- An example of asymptotic simplification

Modelling

Classical results of asymptotics

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A tale of two examples (back to PDE theory)

Conservation equation. Let ρ be a density and $\omega \subset \mathbb{R}^d$ any control volume, if \mathbf{j} is the out-going flux

$$\frac{d}{dt} \int_{\omega} \rho \, dx = - \int_{\partial\omega} \mathbf{j} \cdot \mathbf{n} \, dS = - \int_{\omega} \operatorname{div} \mathbf{j} \, dx$$

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Notice $\Delta \varphi(\rho) = \operatorname{div}(\varphi'(\rho) \nabla \rho)$ so $U''(\rho) = \frac{\varphi'(\rho)}{\rho}$.

Consider N with positions X_i of equal masses $1/N$

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Diffusion can added to the particle system by introducing noise [Details](#).

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Keller-Segel ($d = 2$)	$\rho \log \rho$	0	$-\frac{1}{2\pi} \log x $
Swarming / Herding	0	0	$\frac{1}{a} x ^a - \frac{1}{b} x ^b$

In conservation laws, we expect $\int_{\mathbb{R}^d} \rho(t) = \int_{\mathbb{R}^d} \rho_0$
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Sometimes mass is not conserved, and we will give an example later.

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Classical results of asymptotics

Calculus of Variations approach

A tale of two examples (back to PDE theory)

It admits a solution

$$K(t, x) = \frac{1}{(4\pi t)^{\frac{d}{2}}} e^{-\frac{|x|^2}{4t}}$$

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- ▶ Any solution satisfies

$$\|\rho(t, \cdot) - K(t, \cdot)\|_{L^1} \rightarrow 0 \quad \text{as } t \rightarrow \infty.$$

This is known as **asymptotic simplification**.

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- **[Brezis and Friedman 1983]** proved that δ_0 does not diffuse:
if we take a sequence $\rho_j(0^+, \cdot) \rightarrow \delta_0$, the associated solution $\rho_j(t) \rightarrow \delta_0$.

Notice that the heat kernel is **self-similar**

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A similar approach works for the Porous Medium Equation, where the profile is B .

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For $d \geq 2$ we can write $v = W * u$ for W the Newtonian potential.

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There exists $M^* > 0$ such that

- ▶ If $M < M^*$ solutions are global-in-time.
- ▶ If $M > M^*$ there is finite-time blow-up. And $\rho(T^*) = M\delta_0$.

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When $M > M^*$ there exist $\|\rho_0\|_{L^1} = M$ such that $\mathcal{F}[\rho_0] < 0$.

For

$$\frac{\partial \rho}{\partial t} = \operatorname{div} \left(\rho \nabla (U'(\rho) + V + W * \rho) \right) \quad (\text{ADE})$$

can we classify characterise ρ_∞ such that

$$\rho(t) \rightarrow \rho_\infty$$

in terms of general U, V, W ?

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A tale of two examples (back to PDE theory)

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If $D^2F \geq \lambda I$ then $|X(t) - X_\infty| \leq e^{-\lambda t} |X_0 - X_\infty|$.

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We can rewrite the Heat Equation

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In general, the $\nabla_{L^2} \mathcal{F}$ is given by the Euler-Lagrange equations [► Details](#)

Our equations are “nice” in 2-Wasserstein space (\mathcal{P}_2) . [▶ Details](#)

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The precise definition of solution is the notion of *curves of maximal slope*. [▶ Details](#)

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Due to the estimate above, at an minimiser ρ_∞ , we have

$$\rho_\infty \nabla \frac{\delta \mathcal{F}}{\delta \rho} [\rho_\infty] = 0.$$

Either $\rho_\infty = 0$ (as in PME), or $\frac{\delta \mathcal{F}}{\delta \rho} [\rho_\infty] = C$ (over open sets).

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This gives the intuition that for $M > 8\pi$ then δ_0 (i.e. $\lambda \rightarrow \infty$) is energy beneficial.

Free-energy minimisation for (ADE) when $V = 0$

Existence and non-existence of δ_0

Minimisation for $U = \frac{m}{m-1} \rho^m$, $V = 0$, and $W(x) = |x|^\lambda / \lambda$:

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- Numerical results for $\lambda = 2k$

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$m \in (0, 1)$, $W = 0$ and V radially non-decreasing

The Euler-Lagrange equation is

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The question is

$$\rho(t) \rightarrow \rho_\infty?$$

Outside the displacement convex range, we have to go back to PDE methods.

[Cao and Li 2020]: If $\rho_{V+h_1} \leq \rho_0 \leq \rho_{V+h_2}$ with $h_1, h_2 > 0$ then L_{loc}^∞ convergence to

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Then $\exists \rho_0 \in L^1(\mathbb{R}^d)$ such that $\forall r > 0$

$$M(t, r) = \int_{B_r} \rho(t, x) \, dx \nearrow \int_{B_r} \rho_V(x) \, dx + \underbrace{1 - \|\rho_V\|_{L^1}}_{\text{a Dirac!}} \quad \text{with } a > 0 \text{ as } t \rightarrow \infty.$$

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The key idea is that M satisfies a Hamilton-Jacobi type equation.

► Sketch of Proof

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Remark

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If $W \in L^\infty(\mathbb{R}^d)$ and $\rho \in L^1(\mathbb{R}^d)$, then $W * \rho \in L^\infty(\mathbb{R}^d)$.

The Euler-Lagrange equation is $\log \rho + W * \rho = c$, so

$$\rho = e^c e^{W * \rho} \geq e^c e^{-\|W * \rho\|_{L^\infty}} > 0.$$

Therefore, in this range we always expect diffusion.

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[Cañizo, Carrillo, and Schonbek 2012]: for small W :

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Theorem [Carrillo, G-C, Yao, and Zeng 2021] [Sketch of proof](#)

Let $n \geq 2$, and assume $W(x) = W(-x)$

- ▶ $W \in \mathcal{W}^{1,\infty}(\mathbb{R}^d)$
- ▶ $\nabla W \in L^{n-\varepsilon}(\mathbb{R}^d)$
- ▶ $\Delta W \in L^{\frac{n}{2}}(\mathbb{R}^d)$ (and also $\Delta W \in L^{\frac{n}{2}-\varepsilon}(\mathbb{R}^d)$ if $n \geq 3$)

Then (\star) .

Notice that this hypothesis work for $W(x) \sim |x|^{-\varepsilon}$ for any $\varepsilon > 0$,
but not for the critical case $W(x) \sim \log |x|$.

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2. Does it work for some classes $W \neq 0$.

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2. Does it work for some classes $W \neq 0$.

The answer seems positive for some W .

PhD plan of Alejandro Fernández-Jiménez (U. Oxford).

Thank you for your attention!



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The heat equation and Brownian motion in $d = 1$

▶ [Go back](#)

Consider an stochastic particle jumping over the mesh $\{\dots, -h, 0, h, 2h, \dots\}$ ($h > 0$).

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This gives rise to the intuition (which has to be understood in terms of the Itô calculus)

$$dX_t = dW_t$$

Consider 1 particle. Using a similar arguments, for the stochastic equation

$$dX_t = \underbrace{\mu(t, X_t)}_{\text{drift}} dt + \underbrace{\sigma(t, X_t)}_{\text{diffusion}} dW_t$$

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its probability density ρ is the solution of the Fokker-Planck equation

$$\frac{\partial \rho}{\partial t}(t, x) = -\operatorname{div}(\mu(t, x)\rho(t, x)) + \Delta(D(t, x)\rho(t, x))$$

where $D = \frac{\sigma^2}{2}$.

Imagine now we have N stochastic particles at positions $X_1(t), \dots, X_N(t)$.
We assume they have equal mass.

Recall the empirical measure $\mu_t^N = \frac{1}{N} \sum_{j=1}^N \delta_{X_j(t)}$

²Convergence in law: pointwise convergence of distribution functions at continuity points of the limit

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$$dX_i = -\frac{1}{N} \sum_{j \neq i} \nabla W(X_i - X_j) - \frac{1}{N} \nabla V(X_i) + \sqrt{2D} dW_t^i$$

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This corresponds to $U(\rho) = D \rho \log \rho$.

Mean-Field Approximation: As $N \rightarrow \infty$

$$\mu_0^N \rightarrow \rho_0 \text{ in the tight topology} \implies \mu_t^N \rightarrow \rho(t) \text{ in law for a.e. } t > 0.$$

For the details see, e.g., [Jabin and Wang 2017].

²Convergence in law: pointwise convergence of distribution functions at continuity points of the limit

Let $\partial_t \rho = \Delta \rho^m$ with $m < \frac{d-2}{d}$ and $d \geq 3$ and $\rho_0 \in L^q(\mathbb{R}^d)$ with $q = \frac{(1-m)d}{2}$:

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$$\frac{d}{dt} \frac{1}{q} \int_{\mathbb{R}^d} \rho^q \stackrel{\text{PDE}}{=} -C \int_{\mathbb{R}^d} |\nabla \rho^{\frac{m+q}{2}}|^2$$

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The equation $\frac{d}{dt} X = -CX^\alpha$ where $\alpha < 1$ has finite time extinction.

Take $\varepsilon > 0$, taking $\rho_0^\varepsilon \in L^q$ with $\|\rho_0 - \rho_0^\varepsilon\|_{L^1} \leq \varepsilon$. For $t \geq T_\varepsilon^*$

$$\|\rho(t)\|_{L^1} \leq \|\rho(t) - \rho^\varepsilon(t)\|_{L^1} + \|\rho^\varepsilon(t)\|_{L^1}$$

Take $\varepsilon > 0$, taking $\rho_0^\varepsilon \in L^q$ with $\|\rho_0 - \rho_0^\varepsilon\|_{L^1} \leq \varepsilon$. For $t \geq T_\varepsilon^*$

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Computation of the Wasserstein gradient

Following [Ambrosio, Gigli, and Savare 2005, §10.4.1] [Go back](#)

\mathcal{P}_2 is not a vector space, so there we are not using the intrinsic notion of Fréchet gradient.

The correct notion is **Fréchet subdifferentials** (we will not define it here).

Also, we can see \mathcal{P}_2 inside the space of measures.

Fix $\rho_0 \in \mathcal{P}_2(\mathbb{R}^d)$. Then, the tangent space is given by

$$\text{Tan}_{\rho_0} \mathcal{P}_2(\mathbb{R}^d) = \left\{ \xi : \exists \zeta_n \in C_c(\mathbb{R}^d, \mathbb{R}) \text{ s.t. } \int_{\mathbb{R}^d} |\xi - \nabla \zeta_n|^2 d\rho_0 \rightarrow 0 \right\}$$

Take $\xi = \nabla \zeta$ with $\zeta \in C_c^\infty(\mathbb{R}^d; \mathbb{R})$. Then, by [Ambrosio, Gigli, and Savare 2005, Lemma 5.5.3]

$$\rho_\varepsilon = (1_{\mathbb{R}^d} + \varepsilon \xi) \# \rho_0 = \frac{\rho_0}{\det(1_{\mathbb{R}^d} + \varepsilon \nabla \xi)} \circ (1_{\mathbb{R}^d} + \varepsilon \xi)^{-1}$$

The map $(x, \varepsilon) \mapsto \rho_\varepsilon(x)$ is C^2 and

$$\lim_{\varepsilon \rightarrow 0} \rho_\varepsilon = \rho_0, \quad \frac{\partial}{\partial \varepsilon} \Big|_{\varepsilon=0} \rho_\varepsilon = -\text{div}(\rho \xi).$$

For ε small enough $1_{\mathbb{R}^d} + \varepsilon \nabla \zeta$ is an optimal transport map, so ρ_ε is a constant-speed geodesic.

Hence, using standard variation formulae (see [Giaquinta and Hildebrandt 1996])

$$\lim_{\varepsilon \rightarrow 0} \frac{\mathcal{F}[\rho_\varepsilon] - \mathcal{F}[\rho_0]}{\varepsilon} = - \int_{\mathbb{R}^d} \frac{\delta \mathcal{F}}{\delta \rho}[\rho_0] \nabla \cdot (\rho \xi) = \int_{\mathbb{R}^d} \nabla \zeta \nabla \frac{\delta \mathcal{F}}{\delta \rho}[\rho_0] d\rho$$

This characterises $\nabla_{d_2} \mathcal{F} = -\text{div}(\rho \nabla \frac{\delta \mathcal{F}}{\delta \rho})$ in a broad distributional sense.

Let

$$\mathcal{F}[\rho] = \int_{\mathbb{R}^d} F(x, \rho(x), \nabla \rho(x)) \, dx.$$

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Expanding $F(x, s, \xi)$ in Taylor expansion yields

$$\lim_{\varepsilon \rightarrow 0} \frac{\mathcal{F}[\rho_0 + \varepsilon \varphi] - \mathcal{F}[\rho_0]}{\varepsilon} = \int_{\mathbb{R}^d} \left(\frac{\partial F}{\partial s}(x, \rho_0, \nabla \rho_0) \varphi + \frac{\partial F}{\partial \xi}(x, \rho_0, \nabla \rho_0) \cdot \nabla \varphi \right)$$

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Thus

$$\nabla_{L^2} \mathcal{F}[\rho_0] = \frac{\delta \mathcal{F}}{\delta \rho}[\rho_0] = \frac{\partial F}{\partial s}[\rho_0] - \operatorname{div} \left(\frac{\partial F}{\partial \xi}[\rho_0] \right).$$

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This is the Euler-Lagrange equation!

Convex functions of a measure

Following [Demengel and Temam 1986]

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Given

$$\mathcal{F}[\rho] = \int_{\mathbb{R}^d} f(\rho) \, dx$$

where $f : \mathbb{R} \rightarrow \mathbb{R}$.

The question is what is the natural lower semicontinuous extension of \mathcal{F} to $\mathcal{M}(\mathbb{R}^d)$ with the weak- \star topology.

Given a measure μ and mollifiers η_ε we define $\rho_\varepsilon = \mu * \eta_\varepsilon$.

For $|f(\xi)| \leq C(1 + |\xi|)$ define

$$f_\infty(\xi) = \lim_{t \rightarrow \infty} \frac{f(t\xi)}{t}.$$

Since we can use the Lebesgue decomposition theorem $\mu = \rho \, dx + \mu^s$, where ρ is the Radon-Nikodym derivative of μ . Then

$$\tilde{F}[\mu] = \int_{\mathbb{R}^d} f(\rho) \, dx + f_\infty(\mu^s).$$

The notion of $f_\infty(\mu^s)$ is tricky (but possible) to define.

If $f(s) = s^m$ with $m < 1$, then $f_\infty = 0$.

Curves of maximal slope

(see [Ambrosio, Gigli, and Savare 2005])

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Typically, $\frac{\partial \rho}{\partial t} = -\nabla_X \mathcal{F}[\rho(t)]$ for $X = L^2, H^1$ is satisfied in the dual sense.

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The main idea is the equivalence for $u : [0, T] \rightarrow \mathbb{R}^d$ that

$$u'(t) = -\nabla \mathcal{F}(u), \quad \Longleftrightarrow \quad \begin{cases} \frac{d}{dt}(\mathcal{F} \circ u) = -|\nabla \mathcal{F}(u)| |u'| & \text{orientation} \\ |u'| = |\nabla \mathcal{F}(u)| & \text{norm} \end{cases}$$

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We define the metric slopes

$$|\mu'| (t) = \limsup_{h \rightarrow 0} \frac{d_2(\mu(t+h), \mu(t))}{h}, \quad |\partial \mathcal{F}|[\mu] = \limsup_{\nu \rightarrow \mu} \frac{(\mathcal{F}[\mu] - \mathcal{F}[\nu])_+}{d_2(\mu, \nu)}$$

Curves of maximal slope

(see [Ambrosio, Gigli, and Savare 2005])

[Go back](#)

Typically, $\frac{\partial \rho}{\partial t} = -\nabla_X \mathcal{F}[\rho(t)]$ for $X = L^2, H^1$ is satisfied in the dual sense.

The way in which $\frac{\partial \rho}{\partial t} = -\nabla_{d_2} \mathcal{F}[\rho(t)]$ is rather tricky since \mathcal{P}_2 is not linear a space.

The main idea is the equivalence for $u : [0, T] \rightarrow \mathbb{R}^d$ that

$$u'(t) = -\nabla \mathcal{F}(u), \quad \Longleftrightarrow \quad \begin{cases} \frac{d}{dt}(\mathcal{F} \circ u) = -|\nabla F(u)| |u'| & \text{orientation} \\ |u'| = |\nabla \mathcal{F}(u)| & \text{norm} \end{cases}$$

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Definition 1 Maximal slope curve

A locally abs. cont. curve $t \mapsto \mu(t) \in \mathcal{P}_2(\mathbb{R}^d)$ such that $t \mapsto \mathcal{F}[\mu(t)]$ is abs. cont. and

$$\frac{1}{2} \int_s^t |\mu'|^2(r) \, dr + \frac{1}{2} \int_s^t |\partial \mathcal{F}|^2[\mu(r)] \, dr \leq \mathcal{F}[\mu(s)] - \mathcal{F}[\mu(t)] \quad \forall 0 \leq s < t \leq T$$

Given a radially decreasing $\rho \geq 0$, $\rho^q \in L^1(B_R)$ for some $q > 0$ (for any $R \leq \infty$), using an old trick of Lieb's (see [Lieb 1977; Lieb 1983]) we get, for $|x| \leq R$,

$$\int_{B_R} \rho^q dx = n\omega_n \int_0^R \rho(r)^q r^{n-1} dr \geq n\omega_n \int_0^{|x|} \rho(r)^q r^{n-1} dr \geq n\omega_n \rho(x)^q \int_0^{|x|} r^{n-1} dr.$$

Hence, we deduce the point-wise estimate

$$\rho(x) \leq \left(\frac{\int_{B_R} \rho^q}{n\omega_n |x|^n} \right)^{\frac{1}{q}}. \quad (1)$$

It is easy to see that (1) is not sharp. However, it is useful to prove tightness for sets of probability measures.

For (DE) **entropy solutions**:

$$\rho_0 \in L^1 \implies \exists! \rho \in C([0, +\infty); L^1(\mathbb{R}^d))$$

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The L^1 framework is not enough!

Total variation: $\|\mu\|_{\mathcal{M}} = |\mu|(\mathbb{R}^d).$

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We want to construct a distance between measures such that

$$d(\delta_a, \delta_b) = |a - b|.$$

Given $\mu, \nu \in \mathcal{P}(X)$, taking plans between μ and ν :

$$\Pi(\mu, \nu) = \left\{ \pi \in \mathcal{P}(X \times Y) : \pi(A \times Y) = \mu(A), \quad \pi(X \times B) = \nu(B) \right\}.$$

we define the p -Wasserstein distance

$$d_p(\mu, \nu) = \left(\inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times X} |x - y|^p \, d\pi(x, y) \right)^{\frac{1}{p}}$$

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The correct space to work with this distance is

$$\mathcal{P}_p(\mathbb{R}^d) = \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} |x|^p \, d\mu(x) < \infty \right\}$$

We endow $\mathcal{P}_p(\mathbb{R}^d)$ with the distance d_p .

For simplicity, we restrict to first bounded domains

$$\begin{cases} \partial_t u = \Delta \rho^m + \operatorname{div}(u \nabla V) & x \in \Omega, t > 0 \\ \partial_n u = \partial_n V = 0 & \partial\Omega. \end{cases}$$

For $m \in (0, 1)$, $V \in W^{1,\infty}$, then the solution is well-defined and regular for all $t > 0$.

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If ρ is radially symmetric, the mass function

$$M(t, r) = \int_{B_r} \rho(t, x) \, dx$$

can be studied as viscosity solution of a Hamilton-Jacobi type equation (see [Crandall, Ishii, and Lions 1992]).

For viscosity solutions many properties are known: stability, C^α regularity, ...

We construct an explicit initial datum ρ_0 such that $\partial_t M \geq 0$.

In the limit $M(t, \cdot) \nearrow M_\infty$, a solution of the mass of Euler-Lagrange and $M_\infty(R_v) = 1$.

There are no solutions of sufficient mass. Therefore $M_\infty(0^+) = a > 0$.

First, we prove well-posedness by Duhamel's formula and that, in rescaled variable

- ▶ If $\nabla W \in L^n(\mathbb{R}^d)$ then $\sup_{\tau \geq 1} \|\tilde{\rho}(\tau, \cdot)\|_{H^1} < \infty$.
- ▶ If $n \geq 2$, $\nabla W \in L^n(\mathbb{R}^d)$ and $\Delta W \in L^{\frac{n}{2}}(\mathbb{R}^d)$ then $\sup_{\tau \geq 1} \|\tilde{\rho}(\tau, \cdot)\|_{C^\alpha} < \infty$
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$$\|\rho(t, \cdot) - K(t, \cdot)\|_{L^1} = \|\tilde{\rho}(t, \cdot) - G(\cdot)\|_{L^1}$$

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$$\rightarrow 0, \quad \text{as } t \rightarrow \infty.$$