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Lagrangian discretization of crowd motion and linear diffusion

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Abstract

We study a model of crowd motion following a gradient vector field, with possibly additional interaction terms such as attraction/repulsion, and we present a numerical scheme for its solution through a Lagrangian discretization. The density constraint of the resulting particles is enforced by means of a partial optimal transport problem at each time step. We prove the convergence of the discrete measures to a solution of the continuous PDE describing the crowd motion in dimension one. In a second part, we show how a similar approach can be used to construct a Lagrangian discretization of a linear advection-diffusion equation, interpreted as a gradient flow in Wasserstein space. We provide also a numerical implementation in 2D to demonstrate the feasibility of the computations.

1 Introduction

In this paper we present an approximation scheme to solve evolution PDEs which have a gradient-flow structure in the space of probability measures $\mathcal{P}(\Omega)$ endowed with the Wasserstein distance W_2 . Here, $\Omega \subset \mathbb{R}^d$ is a given compact domain where the evolution takes place, and the PDE will naturally be complemented by no-flux boundary conditions. The approximation that we present is Lagrangian in the sense that the evolving measure ρ_t will be approximated by an empirical measure of the form $\frac{1}{N} \sum_{i=1}^{N} \delta_{X_i(t)}$ and we will look for the evolution of the points X_i . We will use this approximation to provide an efficient numerical method, based on the most recent developments in semi-discrete optimal transport [4, 10, 9, 2]. Here, "semi-discrete" refers to the fact that the discretization of the diffusion effects in the evolution equation involves computation of the optimal transport plans between an empirical measure and diffuse measures.

Starting from the pioneering work of Otto and Jordan-Kinderlherer-Otto [14, 7] it is well-known that some linear and non-linear diffusion can be expressed in terms of a

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gradient flow in the space $W_2(\Omega)$. More precisely, the Fokker-Planck equation

$$\partial_t \rho - \Delta \rho - \operatorname{div}(\rho \nabla V) = 0$$

is the gradient flow of the energy $E(\rho) := \int \rho \log \rho + \int V d\rho$, and the porous-medium equation

$$\partial_t \rho - \Delta \rho^m - \operatorname{div}(\rho \nabla V) = 0$$

is the gradient flow of the energy $E(\rho) := \int \frac{1}{m-1}\rho^m + \int V d\rho$, Recently, also the limit case $m = \infty$ has been considered, in the framework of crowd motion [12]. In this case, the functional is $E(\rho) := \int V d\rho$ if ρ satisfies the constraint $\rho \leq 1$, and $E(\rho) = +\infty$ otherwise; the corresponding PDE is

$$\begin{cases} \partial_t \rho - \operatorname{div}(\rho v) = 0\\ v = -\nabla p - \nabla V\\ 0 \le \rho \le 1, \ p \ge 0, \ p(1 - \rho) = 0 \end{cases}$$

One can see the appearance of a pressure p accounting for the constraint $\rho \leq 1$. We will come back later to the precise meaning and formulations of this last equation.

Approximation by empirical measures Since any probability measure can be approximated by empirical measures, it is tempting to perform an approximation scheme just by considering the gradient flow of one of the above energy functionals E on the set $\mathcal{P}_N(\Omega)$ of uniform measures on N atoms, and then let $N \to \infty$. Unfortunately, the domain of the above functionals is reduced to absolutely continuous measures, and its intersection with $\mathcal{P}_N(\Omega)$ is empty. The main idea and novelty of this paper is to write $E(\rho) = F(\rho) + \int V \, d\rho$ where F is the entropy or the congestion constraint,

$$\begin{split} F(\rho) &= \int \rho \log \rho \qquad \qquad (\text{linear diffusion}) \\ \text{or } F(\rho) &= \begin{cases} 0 & \text{if } \rho \leq 1 \\ +\infty & \text{if not} \end{cases} (\text{crowd motion, } \mathbf{m} = +\infty), \end{split}$$

and to replace F by its Moreau-Yosida regularization

$$F_{\varepsilon}(\mu) := \inf_{\rho} F(\rho) + \frac{1}{2\varepsilon} W_2^2(\mu, \rho).$$

The energies F_{ε} are finite and well-defined for arbitrary probability measures μ , and converge to F as $\varepsilon \to 0$. More importantly, we will see that it is possible to compute very efficiently $F_{\varepsilon}(\mu)$ when $\mu \in \mathcal{P}_N(\Omega)$. The evolution of the discrete measures is then dealt with by keeping track of the positions of the particles $X = (x_1, \ldots, x_N) \in \mathbb{R}^{Nd}$ in the support of the associated measure $\mu_X = \frac{1}{N} \sum_{i=1}^N \delta_{x_i}$. Thanks to the correspondence between X and μ_X , we can think of F_{ε} as an energy on the space of particle positions too, given by

$$F_{\varepsilon}(x_1, \dots, x_N) = F_{\varepsilon} \left(\frac{1}{N} \sum_{1 \le i \le N} \delta_{x_i} \right)$$
(1.1)

The discrete gradient flow then takes the form of a system of ODEs

$$\begin{cases} \frac{1}{N}\dot{x}_{i}(t) = -\nabla_{x_{i}}F_{\varepsilon_{N}}(x_{1}(t),\dots,x_{N}(t)) - \frac{1}{N}\nabla V(x_{i}(t)), \\ X^{N}(0) = X_{0}^{N}, \end{cases}$$
(1.2)

for a suitable choice of $\varepsilon_N \to 0$. The particles are only coupled by the forces $-\nabla_{x_i} F_{\varepsilon_N}(x_1, \ldots, x_N)$ due to diffusion or to the congestion constraint. Finally, we note that the initial condition can be selected by optimal quantization of the initial density $\rho_0 \in \mathscr{P}(\Omega)$,

$$X_0^N \in \underset{X \in \mathbb{R}^{Nd}}{\operatorname{arg\,min}} W_2^2(\rho_0, \mu_X), \tag{1.3}$$

granting, in many situations, an initial error of approximately $W_2^2(\rho_0, \mu_{X_0^N}) \lesssim (1/N)^{1/d}$.

Convergence In the paper we will present the approximation scheme and prove, in these two cases, the convergence of the curves of empirical measures to the solution of the corresponding PDE, under the assumption that a certain bound on the approximate solutions themselves is satisfied. This assumption is unnatural, and it would be desirable to remove it, or replace it with an assumption on the approximation of the initial data. Yet, this seems to be a non-trivial problem, which is closely related to the general question of the convergence of gradient flows once the functionals Γ -converge. We refer to [15, 18] as classical papers on this question, and we observe that a semi-continuity property on the slopes of the functionals is required, which is in the same spirit of the bounds we need. These required bounds are stronger in the crowd motion case, as the equation is non-linear and stronger compactness is needed, while sligthly weaker in the Fokker-Planck case, which is indeed a linear equation.

We then provide an example where these bounds can be obtained, and it is the one-dimensional setting. We will see that the required bounds will be easily proven in 1D crowd motion setting, and that a non-trivial 1D lemma on distributions which are piecewise Gaussians will allow to handle the Fokker-Planck case. However, we insist that these bounds can be verified numerically in general, which makes the scheme we propose interesting for the approximation in arbitrary dimension.

Possible generalizations Our scheme can be considered as a variant of previous schemes involving Voronoi cells (e.g. [3]) but it is, to the best of our knowledge, the first one to use Laguerre cells (see below in the description), which are objects intrinsically related to the Wasserstein structure of the equation. The use of Laguerre cells, easy to handle via modern computational geometry tools, is now state-of-the-art when the transport cost is quadratic. However, we stress that we only use quadratic transport costs in the computation of the Moreau-Yosida regularization of the diffusion or congestion term, which means that we could a priori think of attacking with the same ideas other PDEs, which have for instance a gradient structure for other distances. We refer for instance to [1] for PDEs induced by a cost functions of the form $c(x, y) = |x - y|^q$ or [13] for the so-called relativistic heat equation.

2 Lagrangian discretization of crowd motion

Formulation of the continuous problem We fix a compact domain $\Omega \subset \mathbb{R}^d$ and a potential $V \in C^1(\mathbb{R}^d)$ bounded from below, e.g. $V \ge 0$. The crowd is described by a probability measure ρ in Ω . Each agent tries to follow the gradient vector field $-\nabla V$ while ensuring that the probability density satisfies the density constraint $\rho \le 1$. Therefore, we introduce the constraint set

$$K = \{ \rho \in \mathscr{P}_{\mathrm{ac}}(\Omega) : \rho \le 1 \}.$$

$$(2.1)$$

There are a few possible ways to express this idea of constrained motion, which are at least formally equivalent. The first version is straightforward, but a bit problematic to formulate rigorously. The mass evolution is expressed by a continuity equation where the driving vector field is the projection of $-\nabla V$ onto the tangent cone of the set K:

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho v) = 0, \quad \rho \in K, \\ v = \prod_{T_\rho K} (-\nabla V), \end{cases}$$
(2.2)

where

$$T_{\rho}K = \Big\{ v \in L^2(\Omega; \mathbb{R}^d) : \operatorname{div}(v) \ge 0 \text{ on } \{\rho = 1\}, \ v \cdot n \le 0 \text{ on } \partial\Omega \cap \{\rho = 1\} \Big\},$$

(note that the boundary conditions on $v \cdot n$ are already included in the equation $\partial_t \rho + \operatorname{div}(\rho v) = 0$ and imply $v \cdot n = 0$ on the support of ρ). Projecting to the tangent cone amounts to subtracting a vector from the normal cone, dual to the tangent cone, thereby leading to

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho v) = 0, & \rho \in K, \\ v = -\nabla V - w, & w \in N_\rho K, \end{cases}$$
(2.3)

where

$$N_{\rho}K = \left\{ \nabla p : p \in H^1(\Omega; \mathbb{R}^d), \ p \ge 0, \ p(1-\rho) = 0 \right\},$$

or, more explicitly,

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho v) = 0, & \rho \in K, \\ v = -\nabla V - \nabla p, \\ p \ge 0, \ p(1-\rho) = 0, \end{cases}$$
(2.4)

where p is to be thought of as a pressure field enforcing the density constraint. Finally, solutions to (2.2) also formally coincide with the gradient flow

$$\begin{cases} \partial_t \rho \in -\partial E(\rho), \\ \rho(0) = \rho_0, \end{cases}$$
(2.5)

with respect to the Wasserstein distance W_2 of the energy functional $E : \mathscr{P}(\Omega) \to \mathbb{R} \cup \{\infty\}$ given by

$$E(\rho) = \int V \,\mathrm{d}\rho + F(\rho), \text{ where } F(\rho) = i_K(\rho) = \begin{cases} 0 & \text{ if } \rho \in K \\ +\infty & \text{ if not.} \end{cases}$$

Discretization As explained in the introduction, our strategy for the numerical solution of the crowd motion is to employ a Lagrangian discretization in space of (2.5), meaning that we consider the time evolution of a probability measure which remains uniform over a set containing N points:

$$\mathscr{P}_N(\mathbb{R}^d) = \left\{ \frac{1}{N} \sum_{i=1}^N \delta_{x_i} : x_i \in \mathbb{R}^d \right\}.$$

Since the intersection between the constraint set $K = \{\rho \in \mathscr{P}_{ac}(\Omega) : \rho \leq 1\}$ and $\mathscr{P}_N(\mathbb{R}^d)$ is empty, we are forced to replace the constraint $\rho \in K$ with a penalization, therefore considering the regularized energy given by

$$E_{\varepsilon}(\rho) = \int_{\Omega} V \,\mathrm{d}\rho + \frac{1}{2\varepsilon} \mathsf{d}_{K}^{2}(\rho) = \int_{\Omega} V \,\mathrm{d}\rho + \frac{1}{2\varepsilon} \min_{\sigma \in K} W_{2}^{2}(\rho, \sigma).$$

Note that $\frac{1}{2\varepsilon} \mathbf{d}_K^2$ is the Moreau-Yosida regularization of the convex indicator function $F = i_K$ of the set K.

The evolution of the discrete measures is dealt with by keeping track of the positions of the particles $X = (x_1, \ldots, x_N) \in \mathbb{R}^{Nd}$, to which corresponds the associated measure $\mu_X = \frac{1}{N} \sum_{i=1}^N \delta_{x_i}$. Thanks to the correspondence between X and μ_X , we can think of E_{ε} as an energy on the space of particle positions too, given by

$$E_{\varepsilon}(X) = E_{\varepsilon}(\mu_X) = \frac{1}{N} \sum_{i=1}^{N} V(x_i) + \frac{1}{2\varepsilon} \mathsf{d}_K^2(\mu_X).$$

The gradient flow then takes the form of a system of ODEs

$$\begin{cases} \frac{1}{N} \dot{X}^{N}(t) = -\nabla E^{N} (X^{N}(t)), \\ X^{N}(0) = X_{0}^{N}, \end{cases}$$
(2.6)

where $E^N = E_{\varepsilon_N}$ for a suitable choice of $\varepsilon_N \to 0$. The initial condition can be selected by optimal quantization as in (1.3).

Given $\mu \in \mathscr{P}_N(\mathbb{R}^d)$, let $\sigma \in K$ be the projection of μ onto K, i.e. a minimizer of

$$\min_{\sigma \in K} W_2^2(\mu, \sigma).$$

Its existence follows by compactness, while its uniqueness and continuity with respect to μ are guaranteed by Proposition 5.2 in [5]. Let also $T : \Omega \to \mathbb{R}^d$ be the (unique) optimal transport map from σ to μ . The cell $L_i = T^{-1}(x_i)$ represents the part of the mass of σ which is attached to the particle x_i . Denoting by $\beta_i(X) = \int_{L_i} x \, d\sigma(x) = \int_{L_i} x \, d\sigma(x) / \int_{L_i} d\sigma(x)$ the barycenter of the cell L_i , Proposition 5.1 gives

$$\nabla_{X_i} F_{\varepsilon}(X_1, \dots, X_N) = \frac{1}{N} (x_i - \beta_i(X)),$$
$$\frac{\partial E^N}{\partial x_i}(X) = -\frac{1}{N} \nabla V(x_i) + \frac{1}{N \varepsilon_N} (\beta_i(X) - x_i),$$

and therefore (2.6) becomes more explicitly

$$\begin{cases} \dot{x}_{i}^{N}(t) = -\nabla V(x_{i}^{N}(t)) + \frac{1}{\varepsilon_{N}} [\beta_{i}(X^{N}(t)) - x_{i}^{N}(t)], \\ X^{N}(0) = X_{0}^{N}. \end{cases}$$
(2.7)

Moreover, Proposition 5.1 shows that $\frac{1}{2\varepsilon} \mathsf{d}_K^2$ is $\frac{1}{\varepsilon}$ -concave, which proves that the vector field $-\nabla E_{\varepsilon}(X)$ is well-defined a.e. and provides several useful properties of the flow of this vector field. In particular, following [17] (slightly adapting the proof of Proposition 2.3), one can prove the existence, for every initial datum, of a solution of $X'(t) \in$ $-\partial^+ E_{\varepsilon}(X(t))$ (where ∂^+ is the superdifferential of semi-concave functions). Solutions of this ODE satisfy a reverse Gronwall inequality which provides $|X_1(t) - X_2(t)| \geq$ $e^{-Ct}|X_1(0) - X_2(0)|$, opposite to what happens for the gradient flows of semiconvex functions: this is not useful for uniqueness purposes, but states that solutions cannot concentrate too much, and in particular we obtain that for a.e. initial datum the flow avoids for a.e. time the non-differentiability set. In particular, we have existence of solutions of $X'(t) = -\nabla E_{\varepsilon}(X(t))$ (in the a.e. sense) for a.e. initial datum. Therefore it is always possible to find $\mu_N(0)$ and X_N that satisfy the hypothesis of the following theorem. However, we insist that the goal of the present paper is to show approximation results, and the existence proof for the "discrete" problem with a finite number of particles is not the core of our analysis, which explains why we do not provide more details about the existence for a.e. initial datum.

Theorem 2.1 (Convergence of the discrete scheme). For every $N \in \mathbb{N}$, let $\varepsilon_N \in (0, \infty)$ and $\mu_N(0) \in \mathscr{P}_N(\mathbb{R}^d)$ be such that

$$\frac{1}{\varepsilon_N} W_2^2(\rho_0, \mu_N(0)) \le C, \qquad \lim_{N \to \infty} \varepsilon_N = 0.$$

Let $X_N \in C^1([0,T], \mathbb{R}^{Nd})$ be a solution of (2.6) or, equivalently, (2.7) and let μ_N : $[0,T] \to \mathscr{P}_N(\mathbb{R}^d)$ be the corresponding curve of measures. Assume that

$$\frac{1}{\varepsilon_N^2} \int_0^T W_2^2 \left(\sigma_N, \sum_{i=1}^N \delta_{\beta_i^N} \right) \mathrm{d}t \le C$$
(2.8)

for some constant independent of N. Then, as $N \to \infty$, $\mu_N \to \rho$ in $C^0([0,T]; W_2(\mathbb{R}^d))$, where ρ is a weak solution to (2.4).

Proof. For simplicity of notation, let us write $\beta_i^N(t)$ in place of $\beta_i(X^N(t))$). Define the time dependent vector valued measures

$$M_N(t) = \sum_{i=1}^N \dot{x}_i^N(t) \frac{1}{N} \delta_{x_i^N(t)} = -\frac{1}{N} \sum_{i=1}^N \left[\nabla V(x_i^N(t)) + \frac{1}{\varepsilon_N} (x_i^N(t) - \beta_i^N(t)) \right] \delta_{x_i^N(t)}.$$

Define also the space-time measures $\mu_N \in \mathscr{M}_+([0,T] \times \Omega)$ and $M_N \in \mathscr{M}([0,T] \times \Omega; \mathbb{R}^d)$ given by

$$\mu_N = \int_0^T \delta_t \otimes \mu_N(t) \,\mathrm{d}t, \qquad M_N = \int_0^T \delta_t \otimes M_N(t) \,\mathrm{d}t.$$

By construction they are such that

$$\partial_t \mu_N(t) + \operatorname{div} M_N(t) = 0, \qquad (2.9)$$

because, for any $\varphi\in C^1_c(\mathbb{R}^d),$ one has

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^d} \varphi \,\mathrm{d}\mu_N(t) = \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{N} \sum_{i=1}^N \varphi(x_i^N(t)) \right) = \frac{1}{N} \sum_{i=1}^N \nabla \varphi(x_i^N(t)) \cdot \dot{x}_i^N(t)$$
$$= \int_{\mathbb{R}^d} \nabla \varphi \cdot \mathrm{d}M_N(t) = -\int_{\mathbb{R}^d} \varphi \,\mathrm{div} \, M_N(t).$$

This also means that they solve the continuity equation

$$\partial_t \mu_N + \operatorname{div} M_N = 0 \tag{2.10}$$

in distributional sense.

The first step is showing that the measures μ_N admit a limit in some sense. This is a consequence of the energy estimate

$$\int_{0}^{T} \left| \frac{\mathrm{d}M_{N}(t)}{\mathrm{d}\mu_{N}(t)} \right|^{2} \mathrm{d}\mu_{N}(t) = \int_{0}^{T} \frac{1}{N} \sum_{i=1}^{N} |\dot{x}_{i}^{N}(t)|^{2} \mathrm{d}t$$

$$= \int_{0}^{T} -\nabla E^{N} (X^{N}(t)) \cdot \dot{X}^{N}(t) \mathrm{d}t$$

$$= \int_{0}^{T} -\frac{\mathrm{d}}{\mathrm{d}t} E^{N} (X^{N}(t)) \mathrm{d}t$$

$$= E^{N} (X^{N}(0)) - E^{N} (X^{N}(T)) \leq E^{N} (X^{N}(0)) \leq C,$$
(2.11)

because then the Benamou-Brenier formula for the W_2 distance

$$W_{2}^{2}(\mu_{N}(t_{0}),\mu_{N}(t_{1})) \leq \int_{t_{0}}^{t_{1}} \left| (t_{1}-t_{0}) \frac{\mathrm{d}M_{N}(t)}{\mathrm{d}\mu_{N}(t)} \right|^{2} \mathrm{d}\mu_{N}(t) \,\mathrm{d}t$$
$$\leq \left(\int_{0}^{T} \int_{\Omega} \left| \frac{\mathrm{d}M_{N}(t)}{\mathrm{d}\mu_{N}(t)} \right|^{2} \mathrm{d}\mu_{N} \,\mathrm{d}t \right) |t_{1}-t_{0}|$$

shows that the functions $[0,T] \to (\mathscr{P}(\Omega), W_2) : t \mapsto \mu_N(t)$ are equi-continuous, since they are all 1/2-Hölder with the same constant. Ascoli-Arzelà then ensures that $\mu_N \to \rho$ in $C([0,T], W_2(\Omega))$, up to a subsequence. In particular, $\mu_N \rightharpoonup \rho$ in $\mathscr{M}_+([0,T] \times \Omega)$.

Next, we show that also the family of measures M_N admits a limit. Indeed,

$$\begin{split} \|M_N\|_{\rm TV} &= \int_0^T \|M_N(t)\|_{\rm TV} \, \mathrm{d}t = \int_0^T \frac{1}{N} \sum_{i=1}^N |\dot{x}_i^N(t)| \, \mathrm{d}t = \frac{1}{N} \sum_{i=1}^N \int_0^T |\dot{x}_i^N(t)| \, \mathrm{d}t \\ &\leq \frac{1}{N} \sum_{i=1}^N \sqrt{T} \left(\int_0^T |\dot{x}_i^N(t)|^2 \, \mathrm{d}t \right)^{1/2} \\ &\leq \sqrt{T} \left(\frac{1}{N} \sum_{i=1}^N \int_0^T |\dot{x}_i^N(t)|^2 \, \mathrm{d}t \right)^{1/2} \\ &\leq \sqrt{TE^N(X^N(0))} \leq \sqrt{TC}, \end{split}$$

and by compactness in the space of measures, they admit a weak limit $M_N \to M$ in $\mathcal{M}([0,T] \times \Omega; \mathbb{R}^d)$.

In particular, the weak convergence of μ_N and M_N is sufficient to pass to the limit (2.10) and infer that

$$\partial_t \rho + \operatorname{div} M = 0.$$

To show that $M \ll \rho$, we will use a few properties of the so-called Benamou-Brenier functional $\mathcal{B}_2 : \mathcal{M}([0,T] \times \Omega) \times \mathcal{M}([0,T] \times \Omega, \mathbb{R}^d) \to \mathbb{R} \cup \{+\infty\}$. These properties are found in Proposition 5.18 of [16]: (i) If $M \ll \mu$, $\mathcal{B}_2(\mu, M) = \int_{[0,T] \times \Omega} \left| \frac{\mathrm{d}M}{\mathrm{d}\mu} \right|^2 \mathrm{d}\mu$. (ii) The functional \mathcal{B}_2 is lower semi-continuous wrt narrow convergence. (iii) $\mathcal{B}_2(\mu, M) < +\infty$ only if $\mu \ge 0$ and $M \ll \mu$. In our case, using the fact that $M_N \ll \mu_N$ and previous computations, we get that

$$\mathcal{B}_2(\mu_N, M_N) = \int_0^T \left| \frac{\mathrm{d}M_N(t)}{\mathrm{d}\mu_N(t)} \right|^2 \mathrm{d}\mu_N(t)$$

is uniformly bounded. Then, by lower semi-continuity, $\mathcal{B}_2(\rho, M)$ is finite. This implies, by the third property of \mathcal{B}_2 that $M \ll \rho$.

Let now σ_N be the projection of μ_N on K and let $T_N : \Omega \to \mathbb{R}^d$ be the optimal transport map $(T_N)_{\#}\sigma_N = \mu_N$. Notice that

$$\begin{aligned} \frac{1}{2\varepsilon_N} W_2^2(\mu_N(t), \sigma_N(t)) &= \frac{1}{2\varepsilon_N} \min_{\sigma \in K} W_2^2(\mu_N(t), \sigma) \le E_{\varepsilon_N}(\mu_N(t)) \le E_{\varepsilon_N}(\mu_N(0)) \\ &\le \int_{\Omega} V \, \mathrm{d}\mu_N(0) + \frac{1}{2\varepsilon_N} W_2^2(\rho_0, \mu_N(0)) \\ &\le \int_{\Omega} V \, \mathrm{d}\rho_0 + \mathrm{Lip}(V) W_2(\rho_0, \mu_N(0)) + \frac{1}{2\varepsilon_N} W_2^2(\rho_0, \mu_N(0)) \le C, \end{aligned}$$

therefore $\sigma_N(t)$ converges to the same limit $\rho(t)$ as $\mu_N(t)$. In particular this means that $\rho(t) \in K$ for all t.

For $\xi \in C^1(\mathbb{R}^d; \mathbb{R}^d)$ we have

$$\int_{\mathbb{R}^d} \xi \cdot \mathrm{d}M_N = -\int_{\Omega} \left(\nabla V(T_N) + \frac{T_N - \mathrm{Id}}{\varepsilon_N} \right) \cdot \xi(T_N) \,\mathrm{d}\sigma_N$$

By Brenier's Theorem and the particular structure of the optimal partial transport problem, we have that

$$T_N = \mathrm{Id} - \nabla \psi_N$$

where $\psi_N : \Omega \to \mathbb{R}$ is a semi-concave function satisfying $\psi_N \leq 0$ and $(1 - \sigma_N)\psi_N = 0$; see [12, Lemma 3.1]. If we introduce the pressure field

$$p_N = -\frac{\psi_N}{\varepsilon_N} \ge 0$$

we have that

$$\frac{T_N - \mathrm{Id}}{\varepsilon_N} = \nabla p_N, \qquad (1 - \sigma_N) p_N = 0$$

We must show that $p_N \rightarrow p$ in $L^2([0,T]; H^1(\Omega))$ to some admissible pressure field. This follows by weak-compactness from the equi-boundedness

$$\int_0^T \int_\Omega |\nabla p_N|^2 \, \mathrm{d}x \, \mathrm{d}t \le C < \infty$$

which we are going to prove now. For every $t \in [0, T]$, which we omit for brevity of notation, we have that

$$\begin{split} W_2^2(\mu_N, \sigma_N) &= \sum_{i=1}^N \int_{L_i} |y - x_i|^2 \, \mathrm{d}\sigma(y) = \sum_{i=1}^N \int_{L_i} |y - \beta_i + \beta_i - x_i|^2 \, \mathrm{d}\sigma(y) \\ &= \sum_{i=1}^N \int_{L_i} |y - \beta_i|^2 \, \mathrm{d}\sigma(y) + \sum_{i=1}^N \frac{1}{N} |\beta_i - x_i|^2 + 2\sum_{i=1}^N \int_{L_i} \langle y - \beta_i \mid \beta_i - x_i \rangle \, \mathrm{d}\sigma(y) \\ &= W_2^2 \left(\sigma_N, \frac{1}{N} \sum_{i=1}^N \delta_{\beta_i} \right) + W_2^2 \left(\mu_N, \frac{1}{N} \sum_{i=1}^N \delta_{\beta_i} \right), \end{split}$$

where in the last step we use that $\int_{L_i} (y - \beta_i) d\sigma(y) = 0$. The first term can be treated with the bound given by Proposition 4.1. For the second term, notice that

$$\frac{1}{\varepsilon^2} \int_0^T W_2^2 \left(\mu_N, \frac{1}{N} \sum_{i=1}^N \delta_{\beta_i} \right) dt = \int_0^T \frac{1}{N} \sum_{i=1}^N \left| \frac{x_i - \beta_i}{\varepsilon} \right|^2 dt$$

$$= \int_0^T \frac{1}{N} \sum_{i=1}^N |\dot{x}_i^N + \nabla V(X_i^N)|^2 dt$$

$$\leq 2 \int_0^T \frac{1}{N} \sum_{i=1}^N (|\dot{x}_i^N|^2 + |\nabla V(X_i^N)|^2) dt$$

$$\leq 2C + 2 \operatorname{Lip}(V)^2 T$$
(2.12)

by (2.11). In conclusion,

$$\int_0^T \int_\Omega |\nabla p_N|^2 \, \mathrm{d}x \, \mathrm{d}t = \frac{1}{\varepsilon^2} \int_0^T \int_\Omega |\nabla \psi_N|^2 \, \mathrm{d}x \, \mathrm{d}t$$
$$= \frac{1}{\varepsilon^2} \int_0^T W_2^2(\mu_N, \sigma_N) \, \mathrm{d}t \le CT + 2C + 2\operatorname{Lip}(V)^2 T.$$

The next step is to show that $p(1-\rho) = 0$. The difficulty is that both σ_N and p_N are converging weakly, which is not sufficient in order to pass to the limit the nonlinear relation $p_N(1 - \sigma_N) = 0$.

For $0 \le t_0 < t_1 \le T$, let us introduce the average pressure

$$p_N^{t_0,t_1}(x) = \int_{t_0}^{t_1} p_N(t,x) \, \mathrm{d}t = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} p_N(t,x) \, \mathrm{d}t.$$

Define also the measures $\lambda_N \in \mathscr{M}_+([0,T])$ given by

$$\lambda_N = \|\nabla p_N(t)\|_{L^2(\Omega)} \cdot \mathscr{L}^1 = \left(\int_{\Omega} |\nabla p_N(t)|^2 \,\mathrm{d}x\right) \cdot \mathscr{L}^1.$$

Their total masses

$$|\lambda_N|([0,T]) = \int_0^T \int_\Omega |\nabla p_N|^2 \,\mathrm{d}\sigma_N \,\mathrm{d}t$$

are uniformly bounded, as previously shown; therefore, up to a subsequence, they converge weakly to a measure $\lambda \in \mathcal{M}_+([0,T])$.

For every N, we split in two pieces the following identity:

$$0 = \int_{t_0}^{t_1} \int_{\Omega} p_N(t) \,\mathrm{d}(1 - \sigma_N(t)) \,\mathrm{d}t$$

= $\int_{t_0}^{t_1} \int_{\Omega} p_N(t) \,\mathrm{d}(1 - \sigma_N(t_0)) \,\mathrm{d}t + \int_{t_0}^{t_1} \int_{\Omega} p_N(t) \,\mathrm{d}(\sigma_N(t_0) - \sigma_N(t)) \,\mathrm{d}t$
= $\int_{\Omega} p_N^{t_0, t_1} \,\mathrm{d}(1 - \sigma_N(t_0)) + \int_{t_0}^{t_1} \int_{\Omega} p_N(t) \,\mathrm{d}(\sigma_N(t_0) - \sigma_N(t)) \,\mathrm{d}t.$

Since $p_N^{t_0,t_1} \xrightarrow{L^2(\Omega)} p^{t_0,t_1}$ and $\sigma_N(t_0) \rightarrow \rho(t_0)$ as $N \rightarrow \infty$ (this convergence being weak covergence of measures, but also in L^2 because of the L^∞ bounds on their densities), the first integral converges to

$$\lim_{N \to \infty} \int_{\Omega} p_N^{t_0, t_1} d(1 - \sigma_N(t_0)) = \int_{\Omega} p^{t_0, t_1} d(1 - \rho(t_0)).$$

At any Lebesgue point t_0 of the map $[0,T] \to L^2(\Omega) : t \mapsto p(t)$ we have $p^{t_0,t_1} \xrightarrow[t_1 \to t_0]{} p(t_0)$, hence

$$\lim_{t_1 \to t_0} \int_{\Omega} p^{t_0, t_1} d(1 - \rho(t_0)) = \int_{\Omega} p(t_0) d(1 - \rho(t_0)).$$

Employing Lemma 2.2, the second integral can be estimated as

$$\begin{split} \left| \int_{t_0}^{t_1} \int_{\Omega} p_N(t) \,\mathrm{d}(\sigma_N(t_0) - \sigma_N(t)) \,\mathrm{d}t \right| &\leq \int_{t_0}^{t_1} \|\nabla p_N(t)\|_{L^2(\Omega)} W_2(\sigma_N(t_0), \sigma_N(t)) \,\mathrm{d}t \\ &\leq C \omega(t_1 - t_0) \int_{t_0}^{t_1} \|\nabla p_N(t)\|_{L^2(\Omega)} \,\mathrm{d}t \\ &\leq C \omega(t_1 - t_0) \left(\int_{t_0}^{t_1} \|\nabla p_N(t)\|_{L^2(\Omega)}^2 \,\mathrm{d}t \right)^{1/2} \\ &= C \omega(t_1 - t_0) \sqrt{\frac{\lambda_N([t_0, t_1])}{t_1 - t_0}}, \end{split}$$

where ω is a continuity modulus for the curve $t \mapsto \sigma_N(t)$ in the Wasserstein space W_2 . Note that the curve $t \mapsto \mu_N(t)$ is uniformly $C^{0,1/2}$ as a consequence of the H^1 estimate $\frac{1}{N}\sum_{i=1}^N \left(\int_0^T |\dot{x}_i^N(t)|^2 dt\right) \leq C$, and that the projection operator is continuous (it is also Hölder continuous on bounded sets, see Section 5 in [5]).

When $N \to \infty$, for almost every t_0 and t_1 we have

$$\lim_{N \to \infty} \sqrt{\frac{\lambda_N([t_0, t_1])}{t_1 - t_0}} \le \sqrt{\frac{\lambda([t_0, t_1])}{t_1 - t_0}},$$

which tends to a finite constant when $t_1 \to t_0$ for a.e. t_0 . If we also consider the factor $\omega(t_1 - t_0)$, we see that the second integral goes to 0 for almost every t_0 when taking the limits $N \to \infty$ and $t_1 \to t_0$, in this order.

Summing up, we have shown that

$$\int_{\Omega} p(t_0) \, \mathrm{d}(1 - \rho(t_0)) = \lim_{t_1 \to t_0} \lim_{N \to \infty} \int_{\Omega} p_N(t_0) \, \mathrm{d}(1 - \sigma_N(t_0)) = 0$$

for almost every $t_0 \in [0, T]$, which proves $p(1 - \rho) = 0$, by the positivity of p.

We can finally show that $M = (-\nabla V - \nabla p)\rho$. Fix $\xi \in C^1([0,T] \times \Omega; \mathbb{R}^d)$. We know that

$$\int_0^T \int_\Omega \xi \cdot \mathrm{d}M_N = -\int_0^T \int_\Omega \left(\nabla V(T_N) + \nabla p_N\right) \cdot \xi(T_N) \,\mathrm{d}\sigma_N \,\mathrm{d}t.$$

The first term passes to the limit because

$$\int_0^T \int_\Omega \nabla V \cdot \xi \, \mathrm{d}\mu_N \to \int_0^T \int_\Omega \nabla V \cdot \xi \, \mathrm{d}\rho$$

For the second term,

$$\begin{aligned} \left| \int_0^T \int_\Omega \nabla p_N \cdot [\xi(T_N) - \xi] \, \mathrm{d}\sigma_N \, \mathrm{d}t \right| &\leq \left(\int_0^T \int_\Omega |\nabla p_N|^2 \, \mathrm{d}\sigma_N \, \mathrm{d}t \right)^{1/2} \\ &\cdot \left(\int_0^T \int_\Omega |\xi(T_N) - \xi|^2 \, \mathrm{d}\sigma_N \, \mathrm{d}t \right)^{1/2} \\ &\leq \left(\int_0^T \int_\Omega |\nabla p_N|^2 \, \mathrm{d}\sigma_N \, \mathrm{d}t \right)^{1/2} \operatorname{Lip}(\xi) W_2(\mu_N, \sigma_N) \to 0, \end{aligned}$$

therefore

$$\lim_{N \to \infty} \int_0^T \int_\Omega \nabla p_N \cdot \xi(T_N) \, \mathrm{d}\sigma_N \, \mathrm{d}t = \lim_{N \to \infty} \int_0^T \int_\Omega \nabla p_N \cdot \xi \, \mathrm{d}\sigma_N \, \mathrm{d}t$$
$$= \lim_{N \to \infty} \int_0^T \int_\Omega \nabla p_N \cdot \xi \, \mathrm{d}x \, \mathrm{d}t$$
$$= \int_0^T \int_\Omega \nabla p \cdot \xi \, \mathrm{d}x \, \mathrm{d}t$$
$$= \int_0^T \int_\Omega \nabla p \cdot \xi \, \mathrm{d}\rho \, \mathrm{d}t.$$

The following lemma is borrowed from [12, Lemma 3.5] (but was first presented in other papers, such as [11]).

Lemma 2.2. Let $\mu_0, \mu_1 \in \mathscr{P}(\Omega)$ be probability measures with densities bounded by 1. Then for all $f \in H^1(\Omega)$ we have that

$$\left| \int_{\Omega} f \, \mathrm{d}(\mu_1 - \mu_0) \right| \le \|\nabla f\|_{L^2(\Omega)} W_2(\mu_0, \mu_1).$$

Remark 2.3. The convergence result can be generalized to handle PDEs involving other terms such as self-interaction involving a $C^{1,1}$ kernel W:

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho v) = 0, & \rho \in K, \\ v = -\nabla V - \nabla W * \rho - w, & w \in N_\rho K, \end{cases}$$

which can be regarded as the gradient flow, in $(\mathscr{P}(\Omega), W_2)$ of the energy

$$E(\rho) = \begin{cases} \int_{\Omega} V(x) \, \mathrm{d}\rho(x) + \int_{\Omega} \int_{\Omega} W(x-y) \, \mathrm{d}\rho(x) \, \mathrm{d}\rho(y) & \rho \in K, \\ \infty & \text{otherwise} \end{cases}$$

In this case, the discretized system becomes

$$\begin{cases} \dot{x}_i^N(t) = -\nabla V(x_i^N(t)) - \frac{1}{N} \sum_{j \neq i} \nabla W(x_i - x_j) + \frac{1}{\varepsilon_N} [\beta_i (X^N(t)) - x_i^N(t)], \\ X^N(0) = X_0^N. \end{cases}$$

Theorem 2.4 (Convergence of the discrete scheme in 1D). Let $\Omega \subset \mathbb{R}$ be an interval (not necessarily bounded). For every $N \in \mathbb{N}$, let $\varepsilon_N = 1/N$ and $\mu_N(0) \in \mathscr{P}_N(\mathbb{R})$ be such that

$$\frac{1}{\varepsilon_N} W_2^2(\rho_0, \mu_N(0)) \le C, \qquad \lim_{N \to \infty} \varepsilon_N = 0.$$

Let $X_N \in C^1([0,T], \mathbb{R}^N)$ be a solution of (2.6) or, equivalently, (2.7) and let μ_N : $[0,T] \to \mathscr{P}_N(\mathbb{R})$ be the corresponding curve of measures. Then, as $N \to \infty$, $\mu_N \to \rho$ in $C^0([0,T]; W_2(\mathbb{R}))$, where ρ is a weak solution to (2.4).

Proof. This is an immediate consequence of Theorem 2.1 and Proposition 4.1, which allows to verify the assumption

$$\frac{1}{\varepsilon_N^2} \int_0^T W_2^2 \left(\sigma_N, \sum_{i=1}^N \delta_{\beta_i} \right) \mathrm{d}t \le C.$$

3 Lagrangian discretization of linear diffusion

The previously presented Lagrangian scheme can be adapted to solve also the advectiondiffusion equation

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho v) = 0, \\ v = -\nabla V - \nabla \log \rho. \end{cases}$$
(3.1)

This equation arises as the gradient flow with respect to W_2 of the energy

$$E(\rho) = \int V \,\mathrm{d}\rho + H(\rho) \text{ where } H(\rho) = \begin{cases} \int_{\Omega} \log \rho \,\mathrm{d}\rho & \rho \ll \mathscr{L}^d \llcorner \Omega, \\ \infty & \text{otherwise,} \end{cases}$$

We adopt the same Lagrangian discretization as before. For the atomic measures μ_N , the entropy (the second term in the energy) is identically $+\infty$, therefore we need to substitute it with a similar functional, in the same manner that we replaced the hard constraint $\rho \in K$ with a penalization. To this end, we consider its Moreau-Yosida regularization

$$H_{\varepsilon}(\rho) = \min_{\sigma \in \mathscr{P}(\Omega)} \frac{1}{2\varepsilon} W_2^2(\rho, \sigma) + H(\sigma).$$

and the new energy becomes $E_{\varepsilon}(\rho) = \int_{\Omega} V \, d\rho + H_{\varepsilon}(\rho)$. Letting $F_{\varepsilon}(x_1, \ldots, x_N) = H_{\varepsilon}(\mu_X)$, the discrete measure $\mu_N(t)$ represented by the particles $X_N(t)$ can then evolve according to the system of ODE as before, namely

$$\begin{cases} \frac{1}{N}\dot{x}_i(t) = -\nabla V(x_i) - \frac{1}{N}\nabla_{x_i}F_{\varepsilon}(X), \\ X^N(0) = X_0^N. \end{cases}$$
(3.2)

Theorem 3.1 (Convergence of the discrete scheme). For every $N \in \mathbb{N}$, let $\varepsilon_N \in (0, \infty)$ and $\mu_N(0) \in \mathscr{P}_N(\mathbb{R}^d)$ be such that

$$\frac{1}{\varepsilon_N} W_2^2(\rho_0, \mu_N(0)) \le C, \qquad \lim_{N \to \infty} \varepsilon_N = 0.$$

Let $X_N \in C^1([0,T], \mathbb{R}^{Nd})$ be a solution of (3.2) and let $\mu_N : [0,T] \to \mathscr{P}_N(\mathbb{R}^d)$ be the corresponding curve of measures. Assume that

$$\frac{1}{\varepsilon_N} \int_0^T W_2^2 \left(\sigma_N, \sum_{i=1}^N \delta_{\beta_i} \right) \mathrm{d}t \to 0.$$

Then, as $N \to \infty$, $\mu_N \to \rho$ in $C^0([0,T]; W_2(\mathbb{R}^d))$, where ρ is a weak solution to (3.1).

Proof. Define as before the vector measures

$$M_{N} = \sum_{i=0}^{N} \dot{x}_{i}^{N}(t) \frac{1}{N} \delta_{x_{i}^{N}(t)}.$$

Together with μ_N , they solve the continuity equation

$$\partial_t \mu_N(t) + \operatorname{div} M_N(t) = 0.$$

Moreover,

$$\begin{split} \int_{0}^{T} \left| \frac{\mathrm{d}M_{N}(t)}{\mathrm{d}\mu_{N}(t)} \right|^{2} \mathrm{d}\mu_{N}(t) &= \int_{0}^{T} \frac{1}{N} \sum_{i=1}^{N} |\dot{x}_{i}^{N}(t)|^{2} \, \mathrm{d}t \\ &= \int_{0}^{T} -\nabla E^{N} (X^{N}(t)) \cdot \dot{X}^{N}(t) \, \mathrm{d}t \\ &= \int_{0}^{T} -\frac{\mathrm{d}}{\mathrm{d}t} E^{N} (X^{N}(t)) \, \mathrm{d}t \\ &= E^{N} (X^{N}(0)) - E^{N} (X^{N}(T)) \leq E^{N} (X^{N}(0)) \leq C, \end{split}$$

so the functions $[0,T] \to (\mathscr{P}(\Omega), W_2) : t \mapsto \mu_N(t)$ are equi-continuous, because they are 1/2-Hölder with the same constant. Ascoli-Arzelà then ensures that $\mu_N \rightharpoonup \mu$, up to a subsequence.

The rest of the proof is similar to the previous one with the following modifications. The measure σ_N minimizing

$$\min_{\sigma \in \mathscr{P}(\Omega)} \int_{\Omega} \log \sigma \, \mathrm{d}\sigma + \frac{1}{2\varepsilon} W_2^2(\mu_N, \sigma)$$

satisfies

$$\sigma_N = c_N e^{-\psi_N/\varepsilon_N} \mathscr{L}^d$$

where ψ_N is the optimal potential from σ_N to μ_N and c_N is a normalization constant. This optimality condition can be recovered from the first variation of the objective functional. This means that

$$\frac{T_N - \mathrm{Id}}{\varepsilon_N} = -\frac{\nabla \psi_N}{\varepsilon_N} = \nabla \log \sigma_N = \frac{\nabla \sigma_N}{\sigma_N}.$$

Passing to the limit E_N in order to get $E = -\nabla V \rho - \nabla \rho$ is now easier because

$$\int_0^T \int_\Omega \nabla V \cdot \xi \, \mathrm{d}\mu_N \to \int_0^T \int_\Omega \nabla V \cdot \xi \, \mathrm{d}\rho$$

as before, while, setting $p_N = \log \sigma_N$ (which is the term which plays a similar role to that of the pressure in the previous section), we have

$$\lim_{N \to \infty} \int_0^T \int_\Omega \nabla p_N \cdot \xi(T_N) \, \mathrm{d}\sigma_N \, \mathrm{d}t = \lim_{N \to \infty} \int_0^T \int_\Omega \nabla p_N \cdot \xi \, \mathrm{d}\sigma_N \, \mathrm{d}t$$
$$= \lim_{N \to \infty} \int_0^T \int_\Omega \nabla \sigma_N \cdot \xi \, \mathrm{d}x \, \mathrm{d}t$$
$$= \int_0^T \int_\Omega \nabla \rho \cdot \xi \, \mathrm{d}x \, \mathrm{d}t,$$

where the first step is justified because

$$\left| \int_0^T \int_\Omega \nabla p_N \cdot \left(\xi(T_N) - \xi \right) \mathrm{d}\sigma_N \, \mathrm{d}t \right| \leq \operatorname{Lip}(\xi) \int_0^T \int_\Omega |\nabla p_N| \cdot |T_N - \operatorname{Id}| \, \mathrm{d}\sigma_N \, \mathrm{d}t$$
$$= \operatorname{Lip}(\xi) \frac{1}{\varepsilon_N} \int_0^T \int_\Omega |\nabla p_N|^2 \, \mathrm{d}\sigma_N \, \mathrm{d}t$$
$$= \operatorname{Lip}(\xi) \frac{1}{\varepsilon_N} \int_0^T W_2^2(\sigma_N, \mu_N) \, \mathrm{d}t \to 0.$$

The last term tends to 0 by writing, again,

$$W_{2}^{2}(\sigma_{N},\mu_{N}) = W_{2}^{2}\left(\sigma_{N},\frac{1}{N}\sum_{i=1}^{N}\delta_{\beta_{i}}\right) + W_{2}^{2}\left(\mu_{N},\frac{1}{N}\sum_{i=1}^{N}\delta_{\beta_{i}}\right).$$

The last term tends to 0 by assumption, and the first term is $O(\varepsilon_N)$ because of (2.12). \Box

Theorem 3.2 (Convergence of the discrete scheme in 1D). Let $\Omega \subset \mathbb{R}$ be a bounded interval. For every $N \in \mathbb{N}$, take a number $\varepsilon_N = 1/N$ and $\mu_N(0) \in \mathscr{P}_N(\mathbb{R})$ such that

$$\frac{1}{\varepsilon_N} W_2^2(\rho_0, \mu_N(0)) \le C, \qquad \lim_{N \to \infty} \varepsilon_N = 0, \quad \lim_{N \to \infty} N^2 \varepsilon_N = +\infty.$$

Let $X_N \in C^1([0,T], \mathbb{R}^N)$ be a solution of (3.2) and let $\mu_N : [0,T] \to \mathscr{P}_N(\mathbb{R})$ be the corresponding curve of measures. Then, as $N \to \infty$, $\mu_N \to \rho$ in $C^0([0,T]; W_2(\mathbb{R}))$, where ρ is a weak solution to (3.1).

Proof. This is an immediate consequence of Theorem 3.1 and Proposition 4.2, which provide

$$\frac{1}{\varepsilon_N} \int_0^T W_2^2 \left(\sigma_N, \sum_{i=1}^N \delta_{\beta_i} \right) \mathrm{d}t \le \frac{1}{N\sqrt{\varepsilon_N}} \to 0.$$

4 Bounds in 1D

In this section we prove that, for both the crowd motion and the linear diffusion discretizations, in one dimension there are bounds on the quantities which are relevant for the application of Theorems 2.1 and 3.1. The results come from a static analysis, in the sense that the evolution equations do not play any role in the estimates.

We begin with the easier case of the crowd motion.

Proposition 4.1. Let $\Omega \subset \mathbb{R}$ be an interval. Let $x_1, \ldots, x_N \in \mathbb{R}$, let μ_N be the corresponding atomic measure, σ_N its W_2 -projection on $\{\rho \in \mathscr{P}(K) : \rho \leq 1\}$ and β_1, \ldots, β_N the barycenters of the Laguerre cells¹ L_1, \ldots, L_N . Then, choosing $\varepsilon = 1/N$,

$$\frac{1}{\varepsilon^2} W_2^2 \left(\sigma_N, \sum_{i=1}^N \delta_{\beta_i} \right) \mathrm{d}t \le \frac{1}{12}.$$

Proof. Each Laguerre cell L_i is an interval of length 1/N and its barycenter is the midpoint. Moreover, σ_N has constant density 1 on every cell L_i , therefore

$$W_2^2\left(\sigma_N, \sum_{i=1}^N \delta_{\beta_i}\right) = \sum_{i=1}^N \int_{L_i} |y - \beta_i|^2 \, \mathrm{d}y = \sum_{i=1}^N \int_{\beta_i - 1/(2N)}^{\beta_i + 1/(2N)} |y - \beta_i|^2 \, \mathrm{d}y$$
$$= N \int_{-1/(2N)}^{1/(2N)} y^2 \, \mathrm{d}y = \frac{1}{12N^2},$$

which gives the claim.

We now pass to the case which is relevant for linear diffusion.

Proposition 4.2. Let $\Omega \subset \mathbb{R}$ be a bounded interval. Let $x_1, \ldots, x_N \in \mathbb{R}$, let μ_N be the corresponding atomic measure, and define, for $\varepsilon > 0$:

$$\sigma_N = \operatorname*{arg\,min}_{\rho \in \mathscr{P}(\Omega)} \frac{1}{2\varepsilon} W_2^2(\mu_N, \rho) + \mathcal{H}(\rho).$$

Let β_1, \ldots, β_N be the barycenters of the Laguerre cells L_1, \ldots, L_N of σ_N . Then we have

$$W_2^2\left(\sigma_N, \sum_{i=1}^N \delta_{\beta_i}\right) \le C(\Omega) \frac{\sqrt{\varepsilon}}{N},$$

where $C(\Omega)$ only depends on the length $|\Omega|$ of Ω .

Proof. Let $\ell_i = |L_i|$ denote the length of the *i*-th Laguerre cell. We fix a parameter $\bar{\ell} \in (0, 1)$ to be specified later and divide the cells in two groups:

- short cells: $S = \{i : \ell_i < \overline{\ell}\};$
- long cells: $L = \{i : \ell_i \ge \overline{\ell}\}.$

 $^{^{1}}L_{i} = T^{-1}(x_{i}) \cap \operatorname{spt}(\sigma_{N})$ where T is the optimal transport plan between σ_{N} and μ_{N}

Notice that $|S| \leq N$ and $|L| \leq 1/\overline{\ell}$. Therefore, using Lemma 4.3 to estimate the contribution of the long cells, we get

$$\begin{split} W_2^2 \bigg(\sigma_N, \frac{1}{N} \sum_{i=1}^N \delta_{\beta_i} \bigg) &= \sum_{i \in S} \int_{L_i} |y - \beta_i|^2 c_N e^{-\psi_N/\varepsilon} \, \mathrm{d}y + \sum_{i \in L} \int_{L_i} |y - \beta_i|^2 c_N e^{-\psi_N/\varepsilon} \, \mathrm{d}y \\ &\leq \sum_{i \in S} \frac{1}{N} \ell_i^2 + \sum_{i \in L} \frac{\varepsilon}{2N} \leq \frac{\bar{\ell}}{N} \sum_{i \in S} \ell_i + \frac{\varepsilon}{2\bar{\ell}N} \\ &\leq \frac{\bar{\ell} |\Omega|}{N} + \frac{\varepsilon}{2\bar{\ell}N} = \frac{3\sqrt{|\Omega|}\sqrt{\varepsilon}}{N}, \end{split}$$

where in the last step we chose $\bar{\ell} = \sqrt{\varepsilon/|\Omega|}$.

Lemma 4.3. Let *L* be a cell of length ℓ , $\sigma = \frac{e^{-\varepsilon^{-1}(y-x)^2} dy}{N \int_L e^{-\varepsilon^{-1}(y-x)^2} dy}$ a Gaussian density with mass 1/N over *L*, and $\beta = N \int_L y d\sigma(y)$ the barycenter of $\sigma \sqcup L$. Then

$$\frac{\int_L e^{-\varepsilon^{-1}(y-x)^2} (y-\beta)^2 \,\mathrm{d}y}{N \int_L e^{-\varepsilon^{-1}(y-x)^2} \,\mathrm{d}y} \leq \frac{\varepsilon}{2N}.$$

Proof. By translating, we may assume that $L = [0, \ell]$. We have to treat separately three cases: $x \leq 0, x \in (0, \ell)$ and $x \geq \ell$. Of course the first and the third are equivalent, so we will only consider two cases. We start with the first one.

Notice that the barycenter β minimizes the function $b \mapsto \int_L e^{-\varepsilon^{-1}(y-x)^2} (y-b)^2 dy$, therefore we can bound our original integral with

$$\frac{\int_L e^{-\varepsilon^{-1}(y-x)^2}(y-\beta)^2 \,\mathrm{d}y}{\int_L e^{-\varepsilon^{-1}(y-x)^2} \,\mathrm{d}y} \le \frac{\int_L e^{-\varepsilon^{-1}(y-x)^2}y^2 \,\mathrm{d}y}{\int_L e^{-\varepsilon^{-1}(y-x)^2} \,\mathrm{d}y}$$

by taking b = 0.

Now consider the two functions

$$f(t) = \frac{e^{-\varepsilon^{-1}(t-x)^2}}{\int_L e^{-\varepsilon^{-1}(y-x)^2} \, \mathrm{d}y} \qquad g(t) = \frac{e^{-\varepsilon^{-1}t^2}}{\int_L e^{-\varepsilon^{-1}y^2} \, \mathrm{d}y}$$

They both have integral 1 over the interval L and, if we take $0 \le s \le t \le \ell$, we have that

$$\frac{f(t)}{f(s)} = e^{-\varepsilon^{-1}(t-x)^2 + N(s-x)^2} = e^{-\varepsilon^{-1}t^2 + Ns^2 + 2Nx(t-s)} \le e^{-\varepsilon^{-1}t^2 + Ns^2} = \frac{g(t)}{g(s)}.$$

This means that we can apply Lemma 4.4 with $\varphi(y) = y^2$ and obtain

$$\frac{\int_0^\ell e^{-\varepsilon^{-1}(y-x)^2} y^2 \,\mathrm{d}y}{\int_0^\ell e^{-\varepsilon^{-1}(y-x)^2} \,\mathrm{d}y} = \int_0^\ell f(y) y^2 \,\mathrm{d}y \le \int_0^\ell g(y) y^2 \,\mathrm{d}y = \frac{\int_0^\ell e^{-\varepsilon^{-1}y^2} y^2 \,\mathrm{d}y}{\int_0^\ell e^{-\varepsilon^{-1}y^2} \,\mathrm{d}y}$$

This last integral can be estimated as

$$\begin{aligned} \frac{\int_0^\ell e^{-\varepsilon^{-1}y^2} y^2 \,\mathrm{d}y}{\int_0^\ell e^{-\varepsilon^{-1}y^2} \,\mathrm{d}y} &= \frac{1}{\int_0^\ell e^{-\varepsilon^{-1}y^2} \,\mathrm{d}y} \int_0^\ell (-\frac{2}{\varepsilon}y) e^{-\varepsilon^{-1}y^2} \left(-\frac{y\varepsilon}{2}\right) \mathrm{d}y\\ &= \frac{1}{\int_0^\ell e^{-\varepsilon^{-1}y^2} \,\mathrm{d}y} \left(\left[-\frac{\varepsilon}{2} e^{-\varepsilon^{-1}y^2} y\right]_0^\ell + \int_0^\ell \frac{\varepsilon}{2} e^{-\varepsilon^{-1}y^2} \,\mathrm{d}y \right) \le \frac{1}{2N}. \end{aligned}$$

Noting that the boundary term after the integration by part is negative, putting together the chain of inequalities, we readily obtain the claim.

Regarding the case $x \in (0, \ell)$, we proceed in a similar fashion. First of all, we have that

$$\frac{\int_L e^{-\varepsilon^{-1}(y-x)^2} (y-\beta)^2 \,\mathrm{d}y}{\int_L e^{-\varepsilon^{-1}(y-x)^2} \,\mathrm{d}y} \le \frac{\int_L e^{-\varepsilon^{-1}(y-x)^2} (y-x)^2 \,\mathrm{d}y}{\int_L e^{-\varepsilon^{-1}(y-x)^2} \,\mathrm{d}y}$$

because the barycenter minimizes the integral. With the change of variables $z = \varepsilon^{-1/2}(y-x)$, these integrals become

$$\frac{\int_{L} e^{-\varepsilon^{-1}(y-x)^{2}}(y-x)^{2} \,\mathrm{d}y}{\int_{L} e^{-\varepsilon^{-1}(y-x)^{2}} \,\mathrm{d}y} = \frac{\int_{-\varepsilon^{-1/2}x}^{\varepsilon^{-1/2}(\ell-x)} e^{-z^{2}}\varepsilon^{2}\varepsilon^{2}\varepsilon^{1/2} \,\mathrm{d}z}{\int_{-\varepsilon^{-1/2}x}^{\varepsilon^{-1/2}(\ell-x)} e^{-z^{2}}\varepsilon^{1/2} \,\mathrm{d}z} = \varepsilon \left(\frac{\int_{-\varepsilon^{-1/2}x}^{\varepsilon^{-1/2}(\ell-x)} e^{-z^{2}}z^{2} \,\mathrm{d}z}{\int_{-\varepsilon^{-1/2}x}^{\varepsilon^{-1/2}(\ell-x)} e^{-z^{2}} \,\mathrm{d}z}\right)$$

Letting $a = -\varepsilon^{-1/2}x < 0$ and $b = \varepsilon^{-1/2}(\ell - x) > 0$, an integration by parts shows that

$$\int_{a}^{b} e^{-z^{2}} z^{2} \, \mathrm{d}z = \left[-\frac{e^{-z^{2}} z}{2} \right]_{a}^{b} + \frac{1}{2} \int_{a}^{b} e^{-z^{2}} \, \mathrm{d}z < \frac{1}{2} \int_{a}^{b} e^{-z^{2}} \, \mathrm{d}z,$$

therefore the term in parenthesis is less than 1/2.

Lemma 4.4. Let $I \subset \mathbb{R}$ be an interval and $f, g : I \to [0, \infty)$ two measurable functions such that

$$\int_{I} f(x) \, \mathrm{d}x = \int_{I} g(x) \, \mathrm{d}x = 1$$

and

$$rac{f(y)}{f(x)} \leq rac{g(y)}{g(x)}$$
 for all $x \leq y$ in I .

Then $F(t) \ge G(t)$ for all $t \in I$, where F and G are the cumulative distribution functions of f and g.

Moreover,

$$\int_{I} \varphi(x) f(x) \, \mathrm{d}x \le \int_{I} \varphi(x) g(x) \, \mathrm{d}x$$

for every weakly increasing function $\varphi: I \to \mathbb{R}$.

Proof. Fix $t \in I$ and set $\lambda = f(t)/g(t)$. Then for all $x \leq t \leq y$ we have

$$\frac{f(x)}{g(x)} \ge \lambda \ge \frac{f(y)}{g(y)}.$$

Integrating the first inequality on $I \cap (-\infty, t]$ we get

$$F(t) = \int_{I \cap (-\infty,t]} f(x) \, \mathrm{d}x \ge \lambda \int_{I \cap (-\infty,t]} g(x) \, \mathrm{d}x = \lambda G(t);$$

integrating the second we get

$$1 - F(t) = \int_{I \cap (t,\infty)} f(x) \, \mathrm{d}x \le \lambda \int_{I \cap (t,\infty]} g(x) \, \mathrm{d}x = \lambda [1 - G(t)].$$

Therefore

$$\frac{F(t)}{G(t)} \ge \lambda \ge \frac{1 - F(t)}{1 - G(t)},$$

which translates into

$$\frac{F(t)}{1-F(t)} \ge \frac{G(t)}{1-G(t)}.$$

Since the function $z \mapsto \frac{z}{1-z}$ is strictly increasing in the interval [0, 1], this is equivalent to $F(t) \ge G(t)$.

As a consequence we get that $G^{-1}(F(t)) \ge t$ for all $t \in I$. Finally, if $\varphi : I \to \mathbb{R}$ is weakly increasing, then

$$\int_{I} \varphi(x) f(x) \, \mathrm{d}x \leq \int_{I} \varphi(G^{-1}(F(x))) f(x) \, \mathrm{d}x = \int_{I} \varphi(x) g(x) \, \mathrm{d}x.$$

5 Numerical scheme

5.1 Computation of the Moreau-Yosida regularization

Let $F : \mathscr{P}_{\mathrm{ac}}(\Omega) \to \mathbb{R} \cup \{+\infty\}$, which we assume to be lower-semicontinuous with respect to the Wasserstein metric W_2 . We consider the Moreau-Yosida regularization

$$F_{\varepsilon}: X \in \mathbb{R}^{Nd} \mapsto \inf_{\sigma \in \mathscr{P}_{\mathrm{ac}}(\Omega)} \frac{1}{2\varepsilon} W_2^2(\sigma, \mu_X) + F(\sigma), \tag{5.1}$$

and we assume that for every $X \in \mathbb{R}^{Nd}$, the minimization problem defining $F_{\varepsilon}(X)$ admits a unique solution. We let $\mathcal{D}_N = \{(x_1, \ldots, x_N) \in \mathbb{R}^{Nd} \mid x_i = x_j \text{ for some } i \neq j\}$. Our first proposition gives an explicit formulation for the gradient of $\mathcal{H}_{\varepsilon}$ given a solution σ of the minimization problem defining $\mathcal{H}_{\varepsilon}$.

Proposition 5.1. F_{ε} is $\frac{1}{2N\varepsilon}$ -semiconcave on \mathbb{R}^{Nd} and continuously differentiable on $\mathbb{R}^{Nd} \setminus \mathcal{D}_N$. Given $X = (x_1, \ldots, x_N) \in \mathbb{R}^{Nd} \setminus \mathcal{D}_N$, we let σ the unique minimizer in (5.1), T the unique optimal transport map between σ and μ_X , and $L_i = T^{-1}(x_i)$. Then,

$$\nabla_{x_i} F_{\varepsilon}(X) = \frac{1}{N} \frac{x_i - \beta_i(X)}{\varepsilon} \text{ where } \beta_i(X) := N \int_{L_i} x \, \mathrm{d}\sigma(x)$$

Proof. Let $X \in \mathbb{R}^{Nd}$, σ the unique minimizer in (5.1) and T the unique optimal transport map between σ and μ_X . Given $Y \in \mathbb{R}^{Nd}$,

$$F_{\varepsilon}(Y) \leq \frac{1}{2\varepsilon}W_2^2(\sigma, \delta_Y) + F(\sigma).$$

By construction, one can decompose $\sigma = \sum_{1 \leq i \leq N} \sigma_i$ where $(\sigma_i)_{1 \leq i \leq N}$ are non-negative measures such that $\operatorname{spt}(\sigma_i) \subseteq T^{-1}(\{y_i\})$ and $\sigma_i(\Omega) = 1/N$. Considering the transport which maps σ_i to y_i one gets

$$F_{\varepsilon}(Y) \leq \frac{1}{2\varepsilon} \sum_{i} \int |x - y_{i}|^{2} d\sigma_{i} + F(\sigma)$$

$$\leq \frac{1}{2\varepsilon} \sum_{i} \int |x - x_{i} + x_{i} - y_{i}|^{2} d\sigma_{i} + F(\sigma)$$

$$\leq F_{\varepsilon}(X) + \sum_{i} \langle \frac{1}{N\varepsilon} (\beta_{i} - x_{i}) |x_{i} - y_{i} \rangle + \frac{1}{2N\varepsilon} \sum_{i} |x_{i} - y_{i}|^{2}$$

where we have set $\beta_i = N \int x \, d\sigma_i$. This shows that F_{ε} is $\frac{1}{2N\varepsilon}$ -concave, but also that $\frac{1}{N\varepsilon}(\beta_1 - x_1, \dots, \beta_N - x_N)$ belongs to the superdifferential of F_{ε} at X. If $X \notin D_N$, then $\sigma_i = \sigma|_{T^{-1}(x_i)}$ and the point $\beta_i(X)$ is uniquely defined (we use here the hypothesis on the uniqueness of the minimal σ in (5.1)). Using the stability of optimal transport maps, we get that $X \in \mathbb{R}^{Nd} \setminus D \mapsto \beta_i(X)$ is continuous, which shows that $F_{\varepsilon} \in \mathcal{C}^1(\mathbb{R}^{Nd} \setminus D_N)$ and that $\nabla_{y_i} F_{\varepsilon}(X) = \frac{1}{\varepsilon}(x_i - \beta_i(X))$.

The next two propositions explain how to compute the optimal σ in the definition of the Moreau-Yosida regularization in the crowd motion and linear diffusion. Using Kantorovich duality, this problem can be reformulated as the computation of a Kantorovich potential satisfying a finite-dimensional non-linear system, (5.2) or (5.3).

Given $x_1, \ldots, x_N \in \mathbb{R}^d$ and $\psi \in \mathbb{R}^N$ we define the Laguerre cell of the point y_i as

$$L_{i}(\psi) = \{x \in \mathbb{R}^{d} \mid \forall j, \|x - y_{i}\|^{2} + \psi_{i} \leq \|x - y_{i}\|^{2} + \psi_{i}\}.$$

Proposition 5.2. Consider $F : \mathscr{P}(\Omega) \to \mathbb{R}$ defined by $F(\mu) = 0$ if $\mu \in K$ and $F(\mu) = +\infty$ otherwise, where K is defined in (2.1). Then for all $X \in \mathbb{R}^{Nd} \setminus \mathcal{D}_N$, there exists $\psi \in \mathbb{R}^N_-$ such that

$$\forall i, \ \operatorname{Leb}(L_i(\psi) \cap \Omega \cap \mathcal{B}(y_i, \sqrt{-\psi_i})) = \frac{1}{N}$$
(5.2)

Given such a ψ , define $\varphi = \min(\min_i \|\cdot - x_i\|^2 + \psi_i, 0)$ and $\sigma = \mathbf{1}_{\{\varphi < 0\} \cap \Omega}$.

- (a) $\sigma \in \mathscr{P}_{ac}(\Omega)$ is the Wasserstein projection of μ_X on K,
- (b) $\varphi \leq 0, \ \varphi(1-\sigma) = 0$

(c) (φ, ψ) is an admissible pair of Kantorovich potential in the transport from σ to μ_X Proof. By Kantorovich duality, one can write for any $\sigma \in \mathscr{P}_{ac}(\Omega)$,

$$W_{2}^{2}(\sigma,\mu_{X}) = \max_{\psi \in \mathbb{R}^{N}} \int_{\Omega} \min_{i} ||x - x_{i}||^{2} + \psi_{i} \, \mathrm{d}\sigma(x) - \sum_{1 \le i \le N} \frac{\psi_{i}}{N}$$
$$= \max_{\psi \in \mathbb{R}^{N}} \sum_{1 \le i \le N} \int_{L_{i}(\psi)} ||x - x_{i}||^{2} + \psi_{i} \, \mathrm{d}\sigma(x) - \sum_{1 \le i \le N} \frac{\psi_{i}}{N},$$

thus giving

$$\min_{\sigma \in K} \frac{1}{2\varepsilon} W_2^2(\sigma, \mu_X) = \min_{\sigma \in K} \max_{\psi \in \mathbb{R}^N} \frac{1}{2\varepsilon} \sum_{1 \le i \le N} \int_{L_i(\psi)} \|x - x_i\|^2 + \psi_i \,\mathrm{d}\sigma(x) - \frac{1}{2\varepsilon} \sum_{1 \le i \le N} \frac{\psi_i}{N}$$

Switching the minimum and the maximum, we get the following dual problem

$$\max_{\psi \in \mathbb{R}^N} \min_{\sigma \in L^1(\Omega), 0 \le \sigma \le 1} \frac{1}{2\varepsilon} \sum_{1 \le i \le N} \int_{L_i(\psi)} \|x - x_i\|^2 + \psi_i \, \mathrm{d}\sigma(x) - \frac{1}{2\varepsilon} \sum_{1 \le i \le N} \frac{\psi_i}{N} = \max_{\psi \in \mathbb{R}^N} F(\psi),$$

where, setting $B_i(\psi) = \{x \in \mathbb{R}^d \mid ||x - x_i||^2 + \psi_i \le 0\},\$

$$F(\psi) = \frac{1}{2\varepsilon} \sum_{1 \le i \le N} \int_{L_i(\psi) \cap \Omega \cap B_i(\psi)} ||x - x_i||^2 + \psi_i \, \mathrm{d}x - \frac{1}{2\varepsilon} \sum_{1 \le i \le N} \frac{\psi_i}{N}$$

With similar arguments as in [9, Theorem 1.1], one can prove that F is concave, C^1 , and that its partial derivatives are $\partial_{\psi_i} F(\psi) = \text{Leb}(L_i(\psi) \cap \Omega \cap B_i(\psi))$. It is easy to see that the maximum is attained in the dual problem, thus proving the existence of $\psi \leq 0$ satisfying (5.2).

Define σ and φ as in the statement, the property $\varphi(1-\sigma)$ is obvious. In addition,

$$\varphi(x) - \psi_i = \min(\min_j ||x - x_j||^2 + \psi_j, 0) - \psi_i \le ||x - x_i||^2,$$

so that the pair (φ, ψ) is admissible in the dual Kantorovich problem (and optimal by construction, since φ coincides with the *c*-transform of ψ on the support of σ). This shows that

$$\begin{split} \frac{1}{2\varepsilon}\mathsf{d}_{K}^{2}(\mu_{X}) &\leq \frac{1}{2\varepsilon}W_{2}^{2}(\sigma,\mu_{X}) = \frac{1}{2\varepsilon}\int\varphi\,\mathrm{d}\sigma - \frac{1}{2\varepsilon}\int\psi\,\mathrm{d}\mu_{X} \\ &\leq \frac{1}{2\varepsilon}\sum_{i}\int_{L_{i}(\psi)\cap\Omega\cap B_{i}(\psi)}\varphi\,\mathrm{d}x - \frac{1}{2\varepsilon}\int\psi\,\mathrm{d}\mu_{X} = F(\psi). \end{split}$$

Since the converse inequality holds by weak duality, we get strong duality, and in particular σ is the solution to the primal problem.

The following proposition, dealing with the linear diffusion case, is obtained in a very similar manner (one can instance use Proposition 8.6 in [16] to get the optimality condition for the dual problem). We also refer the reader to Theorems 3.1–3.2 in [2], where similar results are shown for more general functionals.

Proposition 5.3. Let $H : \mathscr{P}(\Omega) \to \mathbb{R}$ be Boltzmann's functional, and $X \in \mathbb{R}^{Nd} \setminus D_N$. Then, there exists $\psi \in \mathbb{R}^N$ such that

$$\forall i, \ \int_{L_i(\psi)} e^{-\frac{1}{2\varepsilon} (\|x - x_i\|^2 + \psi_i)} \, \mathrm{d}x = \frac{1}{N}$$
(5.3)

Given such a ψ , define $\varphi = \min_i \|\cdot - x_i\|^2 + \psi_i$ and $\sigma = e^{-\frac{\varphi}{\varepsilon}} \mathbf{1}_{\Omega}$. Then,

- (a) $\sigma \in \mathscr{P}_{ac}(\Omega)$ is the unique minimizer of $\min_{\mathscr{P}_{ac}(\Omega)} \frac{1}{2\varepsilon} W_2^2(\cdot, \mu_X) + \mathcal{H}(\cdot)$.
- (b) $\frac{1}{2\varepsilon}\varphi + \log(\sigma) = 0$
- (c) (φ, ψ) is an pair of Kantorovich potentials in the transport from σ to μ_X .

Remark 5.4. In practice, equations (5.2) and (5.3) are solved using the same damped Newton algorithm as in [9]. The cells $L_i(\psi)$ are computed using computational geometry techniques ensuring a near-linear computational time in 2D. The integrals are computed exactly in the crowd motion case, and using quadratures ensuring a negligible numerical error in the linear diffusion case.

Remark 5.5. The computation of the Moreau-Yosida regularization of the congestion constraint and the entropy is implemented in the open-source library sd-ot, which is available at https://github.com/sd-ot. The numerical schemes for crowd motion and linear diffusion are implemented as examples in the Python package.

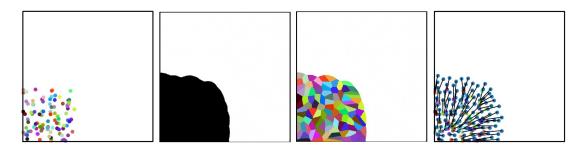


Figure 1: From left to right: a) a point cloud x_1, \ldots, x_N drawn uniformly in $[0, \frac{4}{5}]^2$ with N = 100 points. b) the support of Wasserstein projection of $\mu = \frac{1}{N} \sum_i \delta_{x_i}$ on the set of probability densities bounded by 1, c) the Laguerre cells d) the arrows joining colored points to blue points are proportional to $-\nabla_{x_i} \mathcal{H}_{\varepsilon}(x_1, \ldots, x_N)$.

5.2 Numerical experiments (crowd motion)

In this paragraph, we consider $\Omega \subseteq \mathbb{R}^2$ a compact domain, $V : \Omega \to \mathbb{R}$ a potential, and we define as usual the congestion term $F : \mathscr{P}(\Omega) \to \mathbb{R}$ by $F(\mu) = 0$ if $\mu \leq \text{Leb}$ and $+\infty$ if not. We consider the discretization of the crowd motion model explained above: an initial point set $X^0 = (x_1^0, \ldots, x_N^0)$ is evolved through the ODE system

$$\begin{cases} \frac{1}{N}\dot{x}_i(t) = -\nabla_{x_i}F_{\varepsilon}(x_1(t),\dots,x_{N_h}(t)) - \frac{1}{N}\nabla V(x_i(t)), \\ x_i(0) = x_i^0 \end{cases}$$

which we discretize using a simple explicit Euler scheme:

$$\frac{x_i^{k+1} - x_i^k}{\tau} = -\nabla_{x_i} F_{\varepsilon}(x_1^k, \dots, x_{N_h}^k) - \nabla V(x_i^k).$$

Propositions 5.1–5.2 can be used to compute the gradient of the regularized congestion term F_{ε} . Figure 5.2 illustrates this computation by showing a point set $X = (x_1, \ldots, x_N)$, the projected measure $\sigma \in \mathscr{P}_{ac}(\Omega), \sigma \leq 1$ and the gradient $(\nabla_{x_i} F_{\varepsilon}(X))_{1 \leq i \leq N})$.

Radial case As a first test case, we consider a simple problem with radial symmetry, introduced in [12, Section 5], and whose solution is explicit. The domain is the set $\Omega = \{x \in \mathbb{R}^2 \mid x_2 \geq |x_1|, ||x|| \leq R\}$, and the potential is given by V(x) = ||x||. In our experiment, we assume that R = 2 and $\alpha = \frac{1}{\pi}$, so that $\rho^0 = \alpha \text{Leb}_{\Omega}$ is a probability measure. As shown in [12], the evolution of the crowd is then given by

$$\rho_t(x) = \begin{cases} 1 & \text{if } r \in [0, b(t)] \\ \alpha \left(1 + \frac{t}{\|x\|} \right) & \text{if } r \in [0, b(t)] \\ 0 & \text{if } r \in [R - t, T], \end{cases}$$

where b is a solution of

$$\begin{cases} b(0) = 0\\ b'(t) = \alpha \frac{b(t)+t}{b(t)-\alpha(b(t)+t)}. \end{cases}$$

Given h > 0, we denote $N_h = \text{Card}(\Omega \cap h\mathbb{Z}^2)$ and we let $x_1^0, \ldots, x_{N_h}^0$ be the an arbitrary numbering of the points in the intersection $\Omega \cap h\mathbb{Z}^2$. In all experiments, we set $\tau = \frac{h}{2}$,

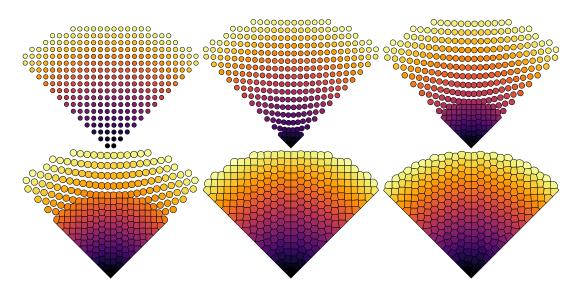


Figure 2: Evolution of particles in the radial case, with $h = \frac{1}{40}$. The color of the cell *i* is related to the position of the point x_i^0 , allowing to visualize the movement of particle.

 $\varepsilon = h$ and T = 1. Figure 5.2 displays the evolution of the Laguerre cells at six time steps. To get error estimates, we measure the Wasserstein distance between:

- $\bar{\rho}_t = (x \mapsto ||x||)_{\#} \rho_t \in \mathscr{P}(\mathbb{R})$, which is the distribution of distances from the origin, computed from the exact solution ρ_t ;
- $\bar{\mu}^k = \frac{1}{N_h} \sum_{1 \le i \le N_h} \delta_{\|x_i^k\|} \in \mathscr{P}(\mathbb{R})$ the distribution of distances from the origin, computed on the discrete solution $\mu^k = \frac{1}{N_h} \sum_{1 \le i \le N_h} \delta_{x_i}$.

The relation between h and $\varepsilon_h = \max_{0 \le k \le \frac{T}{\tau}} W_2(\bar{\rho}_{k\tau}, \bar{\mu}^k)$, as reported in Table 1, suggests a near-linear convergence rate.

h	$\frac{1}{20}$	$\frac{1}{30}$	$\overline{40}$	$\frac{1}{50}$	$\frac{1}{100}$	$\frac{1}{200}$
ε_h	$5.24 \cdot 10^{-2}$	$3.06 \cdot 10^{-2}$	$2.15 \cdot 10^{-2}$	$1.70 \cdot 10^{-2}$	$4.96 \cdot 10^{-3}$	$2.80 \cdot 10^{-3}$

Table 1: Error ε_h between the exact and numeric solution to the crowd motion model as a function of the space-discretization h.

Bimodal case In this case, is obtained as the union of three squares $\Omega = \Omega_{\ell} \cup \Omega_r \cup \Omega_c$: two "rooms" Ω_{ℓ} and Ω_r joined by a corridor Ω_c , where

$$\Omega_{\ell} = [0, \alpha]^2, \quad \Omega_r = [\frac{4}{3}\alpha, \frac{7}{3}\alpha] \times [0, \alpha], \quad \Omega_c = [\alpha, \frac{4}{3}\alpha] \times [\frac{1}{3}\alpha, \frac{2}{3}\alpha], \quad \alpha = \frac{2}{\sqrt{\pi}}$$

The crowd is initially located in the left room Ω_{ℓ} and the potential V is constructed as the distance function to the two corners $\{(\frac{7}{3}\alpha, \alpha), (\frac{7}{3}\alpha, 0)\}$ of the right room Ω_r . More precisely, V is obtained as the solution to the following Eikonal equation, which is computed using a fast marching method:

$$\begin{cases} \|\nabla V\| = 1, \\ V(\frac{7}{3}\alpha, \alpha) = V(\frac{7}{3}\alpha, 0) = 0. \end{cases}$$

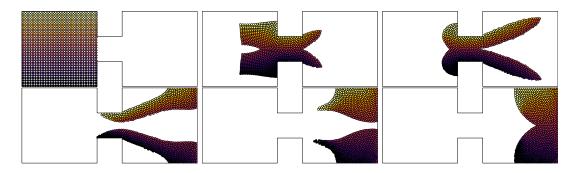


Figure 3: The distribution of the crowd computed at 6 different timesteps, with $h = \frac{\alpha}{30}$. The color of the Laguerre cells encodes the value of the *y* coordinate of the corresponding particle at t = 0.

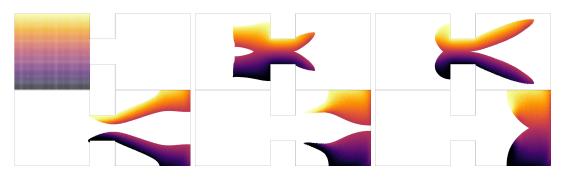


Figure 4: The distribution of the crowd computed at 6 different timesteps, with $h = \frac{\alpha}{80}$.

Given h > 0, we denote $N_h = \text{Card}(\Omega_\ell \cap h\mathbb{Z}^2)$ and we let $x_1^0, \ldots, x_{N_h}^0$ be the list of points in $\Omega_\ell \cap h\mathbb{Z}^2$, so that the crowd is initially located on the left square Ω_ℓ . Here, we set the final time to T = 3, and as before, we have $\varepsilon = h$, $\tau = \frac{h}{2}$.

Visualization In Figures 3 and 4, we visualize the distribution of the crowd at the timesteps $t_i = \frac{i/5}{T}$ for $0 \le i \le 5$, for two space discretizations $h = \frac{\alpha}{30}$ and $h = \frac{\alpha}{80}$. In Figure 5, we highlight some features of the Lagrangian trajectory. First, given a particle x_i^0 , we can compute the minimum time required for the particle to enter the right room:

$$\tau_i := \tau \min\{k \in \mathbb{N} \mid x_i^k \in \Omega_r\}.$$
(5.4)

The exit time τ_i is displayed as a function of the particle coordinate x_i^0 at time t = 0 in the first row of Figure 5. This figure shows (as one could expect) that the exit time is not proportional to the distance to the "door" $\Omega_{\ell} \cap \Omega_c$, as people in front tend to escape faster than those on side of the door. Finally, the next two rows of show the trajectory of the particles. The trajectories seem to be regular in time, but also seem to depend continuously on the initial condition (except near the non-differentiability locus of the potential V).

Remark 5.6 (On the assumption (2.8)). In the 2D cases treated here, we cannot guarantee that our numerical solutions converge to a solution of the crowd motion equation since convergence requires the estimate (2.8). However, it is quite easy to see that this

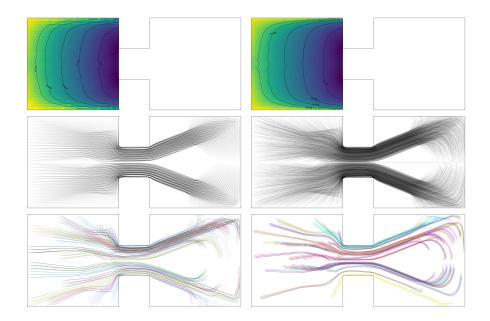


Figure 5: The left (resp. right) column corresponds to $h = \frac{\alpha}{30}$ (resp. $h = \frac{\alpha}{80}$). The first row display the timeout function defined in (5.4), which measures the time taken by a particle to leave the corridor. The second row displays the trajectories of all particles. The third row shows the trajectories of 20 randomly chosen cluster of particles.

estimate holds if one is able to prove that the diameter of the Laguerre cells is bounded uniformly by $C(1/N)^{1/d}$ – this is what is established in 1D in Section 4. Figure 3 (and in fact all our simulations) suggest that such an estimate is satisfied in practice.

Remark 5.7 (Lagrangian interpretation). The Eulerian crowd-motion equation (2.4) can be turned into a Lagrangian equation by introducing the map $s_t \in L^2(\rho_0, \Omega)$, which describes the displacement of the crowd from its position at time t = 0 (more precisely, $s_t(x)$ is the position at time t which was at x at time 0). Formally, s should satisfy the following system

$$\begin{cases} \dot{s} = v \circ s \\ s_0 = \mathrm{id} \\ \rho = s_{\#} \rho_0 \\ v = -\nabla p - \nabla V \\ \rho \le 1, p \ge 0, p(1 - \rho) = 0, \end{cases}$$
(5.5)

and we expect that the numerical solution, shown in Figure 5, provides a piecewiseconstant (in space) approximation to s. We note however that the system (5.5) has not been studied; showing existence of solutions to this system would require to better understand the regularity of the pressure p appearing in (2.4).

5.3 Numerical experiments (diffusion)

In this paragraph, we consider $\Omega \subseteq \mathbb{R}^2$ a compact domain, and we let F be Boltzmann's functional. We consider the discretization of the heat equation explained above: an

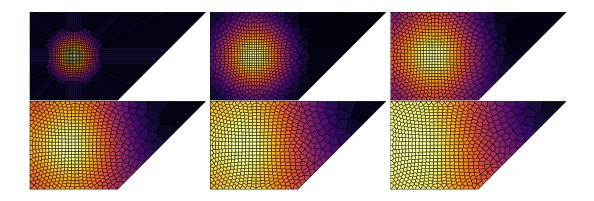


Figure 6: Simulation of the heat equation, at several timesteps, for $h = \frac{1}{30}$. The color of the cell L_i is proportional to $\exp(-\frac{1}{2\varepsilon}(\|\beta_i(X) - x_i\|^2 + \psi_i))$ (see (5.3)). For better visibility, the density is represented on a color scale where the instantaneous maximum is always labeled with the same color (yellow).

initial point set $X^0 = (x_1^0, \ldots, x_N^0)$ is evolved through the ODE system (3.2) (with V = 0), which we discretize again using a simple explicit Euler scheme:

$$\frac{x_i^{k+1} - x_i^k}{\tau} = -\nabla_{x_i} F_{\varepsilon}(x_1^k, \dots, x_{N_h}^k).$$

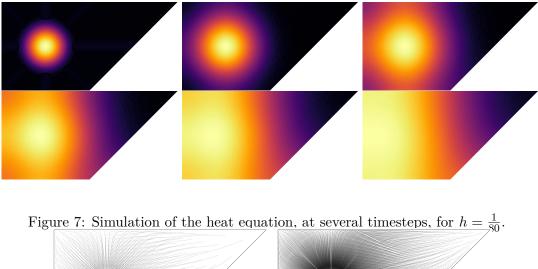
In the numerical example presented in Figures 6,7 and 8, the initial density is uniform over a disk D, and approximated by the uniform measure over $h\mathbb{Z}^2 \cap D$. Despite the lack of convergence result in 2D, one can observe the consistency between the simulations with $h = \frac{1}{30}$ and $h = \frac{1}{80}$.

Remark 5.8 (Lagrangian interpretation). The trajectories we construct (displayed in Figure 8) should not be interpreted as realizations of solutions of the stochastic ODE associated with the heat equation. As in remark 5.7, we expect (but do not prove) that our numerical solutions actually approximate the solution to a Lagrangian equation which can be derived from the heat equation, namely

$$\begin{cases} \dot{s} = v \circ s \\ s_0 = \mathrm{id} \\ \rho = s_{\#} \rho_0 \\ v = -\nabla \log \rho. \end{cases}$$
(5.6)

In contrast with Remark 5.7, the existence of solutions to (5.6) has been established in an article of Evans, Gangbo and Savin [6], assuming that the initial density ρ_0 is bounded from above and below. Their result can also be extended to some non-linear diffusion equations, under assumptions on the nonlinearity. This Lagrangian point of view has already been used to construct numerical schemes for nonlinear diffusion equations, see [8].

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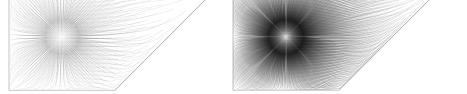


Figure 8: Trajectories of particles along the heat flow (see Rem. 5.8). Left: $h = \frac{1}{30}$, Right: $h = \frac{1}{80}$.

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