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Wasserstein Gradient Flow of the Fisher Information from a Non-Smooth Convex Minimization Viewpoint

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Dedicated to Giuseppe Buttazzo on the occasion of his 70th birthday.

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Motivated by the Derrida-Lebowitz-Speer-Spohn (DLSS) quantum drift diffusion equation, which is the Wasserstein gradient flow of the Fisher information, we study in details solutions of the corresponding implicit Euler scheme. We also take advantage of the convex (but non-smooth) nature of the corresponding variational problem to propose a numerical method based on the Chambolle-Pock primal-dual algorithm.

Keywords: DLSS equation, Wasserstein distance, Fisher information, convex duality, Chambolle-Pock algorithm.

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1. Introduction

The non-linear fourth order parabolic equation

$$\partial_t \rho + \operatorname{div}\Big(\rho \nabla \frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\Big) = 0 \tag{1}$$

appears in the description of interface fluctuations in spin systems [22, 23], as quantum correction to semi-conductor models [2], and in the diffusive limit of a quantum mechanical Boltzmann equation [21]. The mathematical analysis of (1) has been initiated in [8]. By now, well-posedness and long-time asymptotics are fairly well understood.

In the course of the analysis, a remarkable number of structural properties for (1) has been discovered. There exists a whole zoo of integral-type Lyapunov functionals [8, 34], these have been the basis for proving global existence of non-negative weak solutions [28, 35, 36]. Further, the flow induced by (1) is contractive in the Hellinger distance [36], leading to uniqueness of weak solutions [26]. Significant for the paper

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at hand is the observation by Gianazza, Savaré and Toscani that (1) is the (non-convex) gradient flow of the Fisher information in the L^2-Wasserstein distance [28]. Exploiting that gradient flow representation and in particular the intimate relation to the contractive heat flow [17], self-similar long-time asymptotics towards the Gaussian could be proven [42]. Most importantly, the gradient flow formulation of (1) paves the way to the construction of weak solutions by means of the variational JKO scheme [32], see (3) below, both analytically , and, after an additional spatial discretization, also numerically.

In the paper at hand, we derive a novel discrete-in-time variational formulation of (1), prove its unique solvability, and obtain a practical numerical scheme. We thus complement the existing literature both on semi-discretizations [9, 10, 37, 38] and on full discretizations [15, 24, 31, 39, 41, 44] of (1). In comparison to the very sophisticated numerical methods that have been proposed before, our scheme sticks out by simplicity yet robustness. In a nutshell, a time step for (1) is obtained by iterating the following two simple operations: first, the solution of the linear elliptic equation (D_h and $-D_h^*$ denote discrete gradient and divergence, respectively),

$$\phi + \delta D_h^*(\rho_0\, D_h\phi) = f$$

with data ρ_0, an input f from the previous iterate, and a parameter $\delta > 0$; and second, the projection – pointwise at each vertex of the spatial grid – of a certain pair (α, β) of functions defined from the previous iterate to the convex set

$$K = \left\{(a, b) \in \mathbb{R} \times \mathbb{R}^d :\ a + \frac{1}{2}|b|^2 \leq 0\right\}. \tag{2}$$

The parabola K plays a pivotal role in our considerations, since both the Fisher information and the action integral in the dynamical formulation of the Wasserstein metric can be written with the help of K's support function; see Section 2 for further details.

We obtain our time-discrete variational formulation of (1) as dual to the JKO time stepping. We recall the latter: given a time step $\tau > 0$ and an initial datum ρ_0, the semi-discrete approximation ρ_k of the solution to (1) at time $t = k\tau$ is obtained by inductive solution of

$$\rho_k \in \underset{\rho\in\mathscr{P}}{\operatorname{argmin}} \left\{\frac{1}{2\tau}W_2^2(\rho, \rho_{k-1}) + F(\rho)\right\}, \quad F(\rho) = \int \left|\nabla\sqrt{\rho}\right|^2 dx, \tag{3}$$

where W_2 is the L^2-Wasserstein distance. The latter involves the solution of an inner minimization problem, see Section 2 below. The novel dual formulation amounts to choosing $\rho_k \in \mathscr{P}$ such that $\nabla \log \rho_k = \beta_k$, where

$$(\alpha_k, \beta_k) \in \underset{(\alpha,\beta)\in K}{\operatorname{argmax}} \int \left(\frac{\tau}{2}\big(\operatorname{div}\beta - \alpha\big)\right)^c \rho_{k-1}. \tag{4}$$

Also this problem involves an inner minimization via the c-transform $(\cdot)^c$, recalled in Section 2.

Our results concern solutions $\rho_k \in \mathscr{P}(\mathbb{T}^d)$ on the flat d-dimensional torus $\mathbb{T}^d := \mathbb{R}^d/\mathbb{Z}^d$. We show that the minimization problem (3) possesses a unique solution ρ_k, and that this solution is positive and classical.

Then we prove that

$$\alpha_k = -\frac{1}{2}|\nabla \log \rho_k|^2 \quad \text{and} \quad \beta_k = \nabla \log \rho_k \tag{5}$$

form the unique solution pair for the maximization problem (4). Finally, we perform a spatial discretization of (4), apply the Chambolle-Pock algorithm [19] for numerical solution, and use the resulting scheme for approximation of solutions to (1).

Convex minimization algorithms have been used extensively for practical implementation of the JKO time stepping for (non-)linear Fokker-Planck and similar second order parabolic equations. The most common algorithm is the augmented Lagrangian method, also known as ADMM for Alternating Direction Method of Multipliers. The first application of ADMM to an optimal transport problem has been proposed in [4] for numerical solution of the dynamic Benamou-Brenier formulation. This approach has then been extended to transport problems with congestion by Buttazzo, Jimenez and Oudet [12], see also [5, 47]. By now, there are plenty of applications of ADMM to JKO discretizations of gradient flows [6]. For gradient flows of functionals involving derivatives of the density, ADMM is unpractical since it involves the solution of auxiliary nonlinear PDEs at each time step. In the specific case of the Fisher information F from above, the Chambolle-Pock algorithm provides a much better alternative: it is easy to implement and requires no regularization of the datum ρ_{k-1}. In particular, densities that vanish on sets of positive measure are admissible data. The price of robustness, however, is a relatively slow speed of convergence.

We briefly review some of the various alternatives to the aforementioned augmented Lagrangian methods for numerical solution of the JKO stepping for Wasserstein gradient flows. On the one hand, there are fully Lagrangian methods for second [7, 16, 24, 27, 30, 33, 43] and also fourth order [18, 46] parabolic equations, that take advantage of the geometry behind mass transport by approximating the Wasserstein distance directly from mass displacement. Specifically for discretization of (1) in one space dimension, a convergent Lagrangian scheme is given in [44], which also preserves several structural properties like the long-time asymptotics. Concerning variational methods for (1) using finite differences, we mention [39], where minimization in the original JKO formulation (3) is carried out by means of Newton's method. The spatial discretization of the Fisher information is performed such that it blows up for vanishing densities, which keeps the Newton iterates in the region where densities are positive and the functional is strictly convex.

A spatial discretization of the JKO scheme by finite elements has been performed in [11, 13], based on an approximation of the Wasserstein metric by an H^{-1}-distance with explicitly [11] or implicitly [13] defined weight. The resulting method is convergent and numerically robust for Fokker-Planck equations, but is apparently difficult to adapt to fourth order equations.

The paper is organized as follows. Preliminaries from the theory of optimal mass transport are gathered in Section 2 below. In Section 3, we prove existence, uniqueness, positivity and smoothness of the minimizer to the JKO scheme (3). Then, in Section 4, the correspondence (5) between (3) and the dual formulation (4) is established. Finally, in Section 5, the dual problem (4) is spatially discretized and numerically solved.

2. Setting and preliminaries

Spaces. Throughout the paper, we will work in the periodic setting, i.e., on the flat d-dimensional torus $\mathbb{T}^d := \mathbb{R}^d/\mathbb{Z}^d$, equipped with the distance

$$\mathrm{dist}(x,y) = \mathrm{dist}(x-y,0) := \min_{k\in\mathbb{Z}^d} |x-y+k|.$$

We denote by $\mathscr{P}(\mathbb{T}^d)$ and $\mathscr{M}(\mathbb{T}^d)$, respectively, the sets of Borel probability measures and of Borel measures on $\mathbb{T}^d$. By abuse of notation, we shall not distinguish between an absolutely continuous measure $\mu \in \mathscr{P}(\mathbb{T}^d)$ and its probability density $\rho \in L^1(\mathbb{T}^d)$.

Wasserstein metric: primal formulation. The L^2-Wasserstein distance $W_2(\mu,\nu)$ between probability measures $\mu,\nu \in \mathscr{P}(\mathbb{T}^d)$ is given by

$$W_2^2(\mu,\nu) := \inf_{\gamma\in\Pi(\mu,\nu)} \int_{\mathbb{T}^d\times\mathbb{T}^d} \mathrm{dist}^2(x,y)\mathrm{d}\gamma(x,y),\ \forall(\mu,\nu)\in\mathscr{P}(\mathbb{T}^d)^2$$

where $\Pi(\mu,\nu)$ denotes the set of transport plans between μ and ν, i.e. the set of probability measures on $\mathbb{T}^d\times\mathbb{T}^d$ having μ and ν as marginals.

Wasserstein metric: dual formulation. The well-known Kantorovich duality formula, c.f. [49], [50], expresses the Wasserstein distance as a maximization problem,

$$\frac{1}{2}W_2^2(\mu,\nu) := \sup\Big\{ \int_{\mathbb{T}^d} \phi\mathrm{d}\mu + \int_{\mathbb{T}^d}\psi\mathrm{d}\nu \ :\ \phi\oplus\psi \le \frac{\mathrm{dist}^2}{2},\ \Big\}$$

where $\phi\oplus\psi$ denotes the separable function $(x,y)\mapsto\phi(x)+\psi(y)$. It is well-known that this dual formulation admits optimal potentials which can be chosen to be c-conjugates of each other, i.e.

$$\phi(x) = \psi^c(x) := \inf_{y\in\mathbb{T}^d}\Big\{\frac{\mathrm{dist}^2(x,y)}{2} - \psi(y)\Big\},\ \forall x\in\mathbb{T}^d,$$
$$\psi(y) = \phi^c(y) := \inf_{x\in\mathbb{T}^d}\Big\{\frac{\mathrm{dist}^2(x,y)}{2} - \phi(x)\Big\},\ \forall y\in\mathbb{T}^d.$$

In particular ϕ and ψ are $\sqrt{d}$-Lipschitz and 1/2-semi-concave, i.e., the (non-periodic) map $x\in\mathbb{R}^d\mapsto\frac{1}{2}|x|^2-\phi(x)$ is convex.

If the pair $(\phi,\psi)=(\phi,\phi^c)$ solves the Kantorovich dual above, one says that ϕ is a Kantorovich potential between μ and ν. This notion is useful when one wants to differentiate W_2^2 with respect to one of its marginals. The following result is well-known in the euclidean case, for the sake of completeness, we give a proof in the periodic case (which is covered by the analysis of McCann for the general Riemannian case [45], see also Cordero-Erausquin [20] for more on the periodic case):

Lemma 2.1. *Let μ and ν be in $\mathscr{P}(\mathbb{T}^d)$ with μ absolutely continuous with respect to the Lebesgue measure and with an a.e. positive density. Then there exists a unique (up to an additive constant) Kantorovich potential ϕ between μ and ν and*

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}W_2^2(\mu+t(\alpha-\mu),\nu)|_{t=0^+} = \int_{\mathbb{T}^d}\phi\mathrm{d}(\alpha-\mu).$$

Proof. Let $\gamma \in \Pi(\mu, \nu)$ and ϕ be respectively an optimal plan, and a Kantorovich potential between μ and ν, then we have:

$$\phi(x) + \phi^c(y) \leq \frac{\operatorname{dist}^2(x,y)}{2}, \ \forall (x,y) \in \mathbb{T}^d \times \mathbb{T}^d \quad \text{with equality on } \operatorname{spt}(\gamma)$$

since ϕ is Lipschitz it is differentiable a.e. hence μ a.e. and dist^2 is superdifferentiable everywhere. Now if $(x,y) \in \operatorname{spt}(\gamma)$ is such that ϕ is differentiable at x, and that q is in the superdifferential of $\frac{1}{2}\operatorname{dist}^2(.,y)$ at x, then

$$\begin{aligned}\phi(x+h) &\leq \frac{\operatorname{dist}^2(x+h,y)}{2} - \phi^c(y) \\ &\leq \frac{\operatorname{dist}^2(x,y)}{2} - \phi^c(y) + q \cdot h + o(h) = \phi(x) + q \cdot h + o(h).\end{aligned}$$

Hence $q = \nabla\phi(x)$, so the superdifferential of $\frac{1}{2}\operatorname{dist}^2(.,y)$ is reduced to the singleton $\nabla\phi(x)$. This means that $\frac{1}{2}\operatorname{dist}^2(.,y)$ is in fact differentiable at x and satisfies $\nabla\phi(x) = \frac{1}{2}\nabla_x \operatorname{dist}^2(x,y)$. Since this holds at any y such that $(x,y) \in \operatorname{spt}\gamma$, disintegrating γ with respect to μ as $\gamma = \mu \otimes \gamma^x$, we get

$$\nabla\phi(x) = \int_{\mathbb{T}^d} \frac{1}{2}\nabla_x \operatorname{dist}^2(x,y) \mathrm{d}\gamma^x(y) \tag{6}$$

for μ-a.e. $x \in \mathbb{T}^d$. But since the right-hand side of (6) only depends on γ, any other Kantorovich potential should satisfy (6) as well, and then should have μ-a.e. and thus also Lebesgue a.e. the same gradient as ϕ. This shows uniqueness of the Kantorovich potential ϕ up to a constant. Now the differentiability claim is easy to deduce, since denoting by ϕ_t ($t \in (0,1]$) a Kantorovich potential between $\mu + t(\alpha - \mu)$ and ν, one has

$$\int_{\mathbb{T}^d} \phi \mathrm{d}(\alpha - \mu) \leq \frac{1}{2t}[W_2^2(\mu + t(\alpha - \mu), \nu) - W_2^2(\mu, \nu)] \leq \int_{\mathbb{T}^d} \phi_t \mathrm{d}(\alpha - \mu)$$

we can normalize ϕ_t and ϕ to have zero mean and then, since cluster points as $t \to 0^+$ of the (uniformly Lipschitz and bounded) family ϕ_t should be Kantorovich potentials between μ and ν, by the uniqueness shown previously, we deduce that ϕ_t in fact converges uniformly to ϕ which shows the desired result. □

Wasserstein metric: dynamic formulation. For later use in the numerical scheme, we also need the dynamical formulation from [4] of optimal transport. For $\rho_0, \rho_1 \in \mathscr{P}(\mathbb{T}^d)$, we have

$$\frac{1}{2}W_2^2(\rho_0, \rho_1) = \inf\left\{\int_0^1 \int_{\mathbb{T}^d} \frac{|\mathfrak{m}_s|^2}{2\rho_s} \mathrm{d}x \, \mathrm{d}s \ : \ \partial_s \rho_s + \operatorname{div}\mathfrak{m}_s = 0\right\}, \tag{7}$$

where the infimum runs over all pairs $(\rho_s, \mathfrak{m}_s)_{s \in [0,1]}$ of weakly continuous curves $\rho_{(\cdot)} : [0,1] \to \mathscr{P}(\mathbb{T}^d)$ with prescribed end points ρ_0 and ρ_1 and $\mathbb{R}^d$-valued Radon measures $\mathfrak{m}$ on $(0,1) \times \mathbb{T}^d$ such that the continuity equation $\partial_s \rho_s + \operatorname{div}\mathfrak{m}_s = 0$ holds in the sense of distribution. The quotient

$$\operatorname{BB}(r, m) := \frac{|m|^2}{2r} \tag{8}$$

inside the integral in (7) is understood as the convex and lower semi-continuous envelope of the respective expression for $r > 0$, which is zero where $r \geq 0$ and $m = 0$, and infinity where either $r < 0$, or $r = 0$ but $m \neq 0$. This ensures in particular non-negativity of the curve ρ_s. For the fully rigorous formulation of (7), we refer to [1, Chapter 8].

Of particular relevance to us is the fact that the quotient BB is the support function of the convex set K from (2) that is to say that

$$\mathrm{BB}(r,m) = \sup_{(a,b)\in K} \{ar + b\cdot m\} \quad \text{for all } (r,m) \in \mathbb{R}\times\mathbb{R}^d. \tag{9}$$

This confirms the claimed convexity and lower semi-continuity of BB. The Legendre transform of BB is thus the indicator function

$$\mathrm{BB}^*(a,b) = \chi_K(a,b) = \begin{cases} 0 & \text{if } (a,b) \in K \\ +\infty & \text{otherwise.} \end{cases}$$

Fisher information. In (3), we have (informally) introduced the Fisher information functional $F\colon \mathscr{M}(\mathbb{T}^d) \to \mathbb{R}\cup\{+\infty\}$ as

$$F(\rho) := \begin{cases} \int_{\mathbb{T}^d} |\nabla\sqrt{\rho}|^2 & \text{if } \rho \geq 0 \text{ and } \sqrt{\rho} \in H^1(\mathbb{T}^d) \\ +\infty & \text{otherwise.} \end{cases} \tag{10}$$

This functional is convex and lower semi-continuous. Note that if we have $\rho \geq 0$ and $\sqrt{\rho} \in H^1(\mathbb{T}^d)$, then $\nabla\rho = 2\sqrt{\rho}\nabla\sqrt{\rho} \in L^1$, and we may write

$$F(\rho) = \frac{1}{4}\int_{\mathbb{T}^d} \frac{|\nabla\rho|^2}{\rho}.$$

The integrand above is to be understood as zero for $\nabla\rho = 0$ and $\rho = 0$, and as $+\infty$ for $\rho = 0$ but $\nabla\rho \neq 0$. In other words, the quotient is again of the type (8), that is, the support function of the parabola K from (2).

This gives rise to the following alternative representation (which can be obtained by similar arguments as in Proposition 5.18 in [49]):

$$F(\rho) = \sup\left\{ \int_{\mathbb{T}^d} \frac{(\alpha - \mathrm{div}\beta)}{2} \mathrm{d}\rho \,:\, (\alpha,\beta)\in C(\mathbb{T}^d)\times C^1(\mathbb{T}^d,\mathbb{R}^d),\ (\alpha,\beta)\in K \right\}. \tag{11}$$

JKO functional. Finally, let $\tau > 0$ and $\rho_0 \in \mathscr{P}(\mathbb{T}^d)$ be given. We are interested in the (convex) minimization

$$\inf_{\rho\in\mathscr{P}(\mathbb{T}^d)} J(\rho) := \frac{1}{2\tau} W_2^2(\rho_0,\rho) + F(\rho). \tag{12}$$

Existence of a minimizer for (12) is easily shown by the direct method. Uniqueness requires more work, see next section, since neither $W^2(\rho_0, .)$ (which is linear if ρ_0 is a Dirac mass) nor F (which is positively homogeneous) is strictly convex.

3. Uniqueness, positivity and regularity of the minimizer

In this section, we prove:

Theorem 3.1. *The minimization problem* (12) *admits a unique solution ρ. Moreover, $\rho \in W^{3,p}(\mathbb{T}^d)$ for every $p \in [1, +\infty)$ ρ is strictly positive, and ρ solves the Euler-Lagrange PDE*

$$\frac{\phi}{\tau} = \frac{1}{2}\Delta \log \rho + \frac{1}{4}|\nabla \log \rho|^2 = \frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}. \tag{13}$$

where ϕ is a Kantorovich potential between ρ and ρ_0.

Notice that $\rho \in W^{3,p}(\mathbb{T}^d)$ for all $p \geq 1$ implies that $\rho \in C^{2,\alpha}(\mathbb{T}^d)$ for every $\alpha \in [0,1]$. Hence all derivatives in (13) are actually classical.

3.1. Approximation

To enforce positivity, given $\delta > 0$ we consider (as in [14] in the context of the TV-JKO scheme) the entropic approximation of (12):

$$\inf_{\rho \in \mathscr{P}(\mathbb{T}^d)} J_\delta(\rho) := \frac{1}{2\tau} W_2^2(\rho_0, \rho) + F(\rho) + \delta \int_{\mathbb{T}^d} \rho \log \rho. \tag{14}$$

Lemma 3.2. *Given $\delta > 0$,* (14) *admits a unique solution ρ_δ, and ρ_δ satisfies $\rho_\delta + \frac{1}{\rho_\delta} \in L^\infty(\mathbb{T}^d)$.*

Proof. Existence follows from weak $*$ compactness and lower semicontinuity of J_δ and uniqueness by strict convexity. If ρ_δ is constant, there is nothing to prove, setting $m := \mathrm{essinf}\rho_\delta$ and $M := \mathrm{essup}\rho_\delta$ we may therefore assume that $m < M$ and our aim is to show $m > 0$ and $M < +\infty$. To do so, consider the two functions $\underline{G}$ and $\overline{G}$ defined by

$$\underline{G}(\alpha) := \int_{\mathbb{T}^d} (\alpha - \rho_\delta)_+, \ \overline{G}(\alpha) := \int_{\mathbb{T}^d} (\rho_\delta - \alpha)_+, \ \forall \alpha \in \mathbb{R}_+.$$

Both $\underline{G}$ and $\overline{G}$ are 1-Lipschitz, $\underline{G}$ is nondecreasing with $= \underline{G}(m) = 0$, $\underline{G}(\alpha) > 0$ for $\alpha > m$, $\overline{G}$ is nonincreasing with $\overline{G}(M) = 0$ and $\overline{G}(\alpha) > 0$ for $\alpha < M$. We can therefore choose sequences $(m_n)_n$ and $(M_n)_n$ such that

$$m < m_n < M_n < M, \ M_n \nearrow M, \ m_n \searrow m, \ \underline{G}(m_n) = \overline{G}(M_n), \ \forall n. \tag{15}$$

With this choice we define the sequence of competitors to ρ_δ by suitably truncating ρ_δ:

$$\mu_n := \min(M_n, \max(m_n, \rho_\delta))$$

by construction μ_n is a probability measure and

$$\|\mu_n - \rho_\delta\|_{L^1} = \underline{G}(m_n) + \overline{G}(M_n) =: 2\varepsilon_n \to 0 \text{ as } n \to \infty.$$

Since by construction $\sqrt{\mu_n}$ is obtained by truncating $\sqrt{\rho_\delta}$, we have $F(\mu_n) \leq F(\rho_\delta)$, the fact that ρ_δ minimizes J_δ thus gives

$$0 \leq \frac{1}{2\tau}[W_2^2(\mu_n, \rho_0) - W_2^2(\rho_\delta, \rho_0)] + \delta \int_{\mathbb{T}^d} \mu_n \log \mu_n - \delta \int_{\mathbb{T}^d} \rho_\delta \log \rho_\delta$$

By Kantorovich duality formula, denoting by ϕ_n a Kantorovich potential ($\sqrt{d}$-Lipschitz and with zero mean, say) between μ_n and ρ_0, the first term in the right-hand side can be bounded from above by

$$\tau^{-1}\int_{\mathbb{T}^d}\phi_n(\mu_n-\rho_\delta)\leq\tau^{-1}\|\phi_n\|_{L^\infty}\|\mu_n-\rho_\delta\|_{L^1}\leq C_d\tau^{-1}\varepsilon_n$$

where C_d is a just a dimensional constant, using this with the convexity of $t\mapsto t\log t$ and the construction of μ^n, we arrive at

$$\begin{aligned}
0&\leq\frac{C_d}{\tau}\varepsilon_n+\delta\int_{\rho_\delta\leq m_n}(m_n\log(m_n)-\rho_\delta\log(\rho_\delta))+\delta\int_{\rho_\delta\geq M_n}(M_n\log(M_n)-\rho_\delta\log(\rho_\delta))\\
&\leq\frac{C_d}{\tau}\varepsilon_n+\delta\Big((1+\log(m_n))\int_{\mathbb{T}^d}(m_n-\rho_\delta)_+-(1+\log(M_n))\int_{\mathbb{T}^d}(\rho_\delta-M_n))_+\Big)\\
&=\varepsilon_n\Big[\frac{C_d}{\tau}+\delta\log(\frac{m_n}{M_n})\Big]
\end{aligned}$$

which since $\varepsilon_n=\underline{G}(m_n)=\overline{G}(M_n)>0$ implies that $\frac{m_n}{M_n}\geq e^{-\frac{C_d}{\tau\delta}}$ preventing m_n to approach 0 and M_n to approach $+\infty$ and thus enabling us to conclude that $m>0$ and $M<+\infty$ (with $\frac{m}{M}\geq e^{-\frac{C_d}{\tau\delta}}$). □

Since $\sqrt{\rho_\delta}\in H^1(\mathbb{T}^d)$, the fact that ρ_δ is bounded and bounded away from 0 implies that ρ_δ, $\frac{1}{\sqrt{\rho}}$ and $\log\rho_\delta$ belong to $H^1(\mathbb{T}^d)\cap L^\infty(\mathbb{T}^d)$ as well. More importantly, it enables us to justify the Euler-Lagrange satisfied by ρ_δ as follows. Thanks to Lemma 2.1, there exists a unique (up to an additive constant) Kantorovich potential ϕ_δ between ρ_δ and ρ_0. Let $\theta\in C^1(\mathbb{T}^d)$ such that $\int_{\mathbb{T}^d}\theta=0$, for $t\in\mathbb{R}$ with $|t|$ small enough $\rho_\delta+t\theta$ is admissible for (14) so that $J_\delta(\rho_\delta+t\theta)$ is minimal at $t=0$. Using Lemma 2.1, we first have

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}W_2^2(\rho_\delta+t\theta,\rho_0)|_{t=0}=\int_{\mathbb{T}^d}\phi_\delta\theta. \tag{16}$$

Moreover, thanks to Lemma 3.2, we can write

$$\begin{aligned}
\nabla\sqrt{\rho_\delta+t\theta}&=\nabla\sqrt{\rho_\delta}+\frac{1}{2}\int_0^t\nabla\Big(\frac{\theta}{\sqrt{\rho_\delta+s\theta}}\Big)\mathrm{d}s\\
&=\nabla\sqrt{\rho_\delta}+\frac{t}{2}\nabla\Big(\frac{\theta}{\sqrt{\rho_\delta}}\Big)+t\varepsilon_t\text{ with }\varepsilon_t\to0\text{ as }t\to0\text{ in }L^2(\mathbb{T}^d).
\end{aligned}$$

whence
$$\frac{\mathrm{d}}{\mathrm{d}t}F(\rho_\delta+t\theta)|_{t=0}=\int_{\mathbb{T}^d}\nabla\sqrt{\rho_\delta}\cdot\nabla\Big(\frac{\theta}{\sqrt{\rho_\delta}}\Big) \tag{17}$$

and since
$$\frac{\mathrm{d}}{\mathrm{d}t}[\int_{\mathbb{T}^d}(\rho_\delta+t\theta)\log(\rho_\delta+t\theta)]|_{t=0}=\int_{\mathbb{T}^d}\log(\rho_\delta)\theta \tag{18}$$

we deduce
$$\int_{\mathbb{T}^d}\Big(\frac{\phi_\delta}{\tau}+\delta\log\rho_\delta\Big)\theta+\int_{\mathbb{T}^d}\nabla\sqrt{\rho_\delta}\cdot\nabla\Big(\frac{\theta}{\sqrt{\rho_\delta}}\Big)=0 \tag{19}$$

for all $\theta\in C^1(\mathbb{T}^d)$ such that $\int_{\mathbb{T}^d}\theta=0$.

In other words there is some constant C_δ such that $\sqrt{\rho_\delta}$ is a weak solution of

$$\frac{\phi_\delta}{\tau} + \delta \log \rho_\delta - \frac{\Delta\sqrt{\rho_\delta}}{\sqrt{\rho_\delta}} = C_\delta$$

up to absorbing this constant in the Kantorovich potential ϕ_δ we thus have

$$\Big(\frac{\phi_\delta}{\tau} + \delta \log \rho_\delta\Big)\sqrt{\rho_\delta} = \Delta\sqrt{\rho_\delta}. \tag{20}$$

By standard elliptic regularity, the fact that $\phi_\delta \in W^{1,\infty}(\mathbb{T}^d)$ implies that $\sqrt{\rho_\delta}$ belongs to $W^{3,p}(\mathbb{T}^d)$ for every $p \in [1, +\infty)$ hence $\sqrt{\rho_\delta}$ (and ρ_δ) belong to $C^{2,\alpha}(\mathbb{T}^d)$ for every $\alpha \in [0, 1)$, in particular $\sqrt{\rho_\delta}$ is a classical solution of (20).

3.2. Proof of Theorem 3.1

We are now in position to prove Theorem 3.1.

Step 1. $\delta \to 0$. Note that if $\mu \in \mathscr{P}(\mathbb{T}^d)$ and $\sqrt{\mu} \in H^1(\mathbb{T}^d)$ then by the Sobolev imbedding $\mu \in L^{q(d)}$ for some $q(d) > 1$ (for $d = 1, 2$ one can take any exponent in $(1, +\infty)$ and for $d \geq 3$ one can take $q(d) = d/(d-2)$) and in particular μ has finite entropy. From the inequality $J(\rho_\delta) + \delta \int_{\mathbb{T}^d} \rho_\delta \log \rho_\delta \leq J(\mu) + \delta \int_{\mathbb{T}^d} \mu \log \mu$ and the fact that $\int_{\mathbb{T}^d} \rho_\delta \log \rho_\delta$ is bounded from below, one readily deduces that $\sqrt{\rho_\delta}$ is bounded in $H^1(\mathbb{T}^d)$ and therefore (up to extracting a vanishing sequence) converges weakly in $H^1(\mathbb{T}^d)$ as $\delta \to 0^+$ (hence strongly in $L^{p(d)}$ for some $p(d) > 2$) to some $\sqrt{\rho}$, and then ρ_δ converges strongly to ρ in $L^{p(d)/2}$ and ρ obviously solves (12). Note also that both $\rho_\delta \log \rho_\delta$ and $\sqrt{\rho_\delta} \log \rho_\delta$ are bounded in L^1 so that

$$\delta \rho_\delta \log \rho_\delta \ \text{ and } \ \delta\sqrt{\rho_\delta} \log \rho_\delta \ \text{ tend to 0 strongly in } L^1. \tag{21}$$

As for the family of Kantorovich potentials ϕ_δ, we already know that $\|\nabla\phi_\delta\|_{L^\infty} \leq \sqrt{d}$ and integrating (20) and using the periodicity of ρ_δ, we get

$$\int_{\mathbb{T}^d} \Big(\frac{\phi_\delta}{\tau} + \delta \log \rho_\delta\Big)\sqrt{\rho_\delta} = 0$$

which, with (21), the fact that $\sqrt{\rho_\delta}$ converges strongly in L^2 to $\sqrt{\rho}$ with $\int_{\mathbb{T}^d} \rho = 1$ and $\max_{[0,1]^d} \phi_\delta - \min_{[0,1]^d} \phi_\delta \leq \sqrt{d}\,\mathrm{diam}([0, 1]^d) = d$ yields a uniform L^∞ bound on ϕ_δ. Thanks to the Arzelà-Ascoli's Theorem, we may assume (after an extraction again) that ϕ_δ converges uniformly to some ϕ which is a Kantorovich potential between ρ and ρ_0. Since $\Delta\sqrt{\rho_\delta}$ converges to $\Delta\sqrt{\rho}$ in H^-1, $\phi_\delta\sqrt{\rho_\delta}$ converges to $\phi\sqrt{\rho}$ in H^1 and recalling (21), we may pass to the limit in (20) and get

$$\frac{\phi}{\tau}\sqrt{\rho} = \Delta\sqrt{\rho}. \tag{22}$$

Step 2. Positivity and regularity of ρ. The announced $W^{3,p}$ regularity of ρ then follows from equation (22) and elliptic regularity. Setting $u = \sqrt{\rho} \in C^{2,\alpha}(\mathbb{T}^d)$, $f = \tau^{-1}\phi \in W^{1,\infty}$, we have $Lu := \Delta u - f_+ u = -f_- u \leq 0$, hence it follows from the strong maximum principle (Theorem 3.5 in [29]) that if u takes the (global minimum) value 0 one should have $u=0$ contradicting $\int_{\mathbb{T}^d} u^2 = 1$. We thus have found a smooth and everywhere strictly positive solution ρ of (12) and shown that it is a classical solution of (13).

Step 3. Uniqueness. If μ solves (12), so does $\frac{\mu+\rho}{2}$ by convexity of F and $W^2(\rho_0, .)$ yielding that $F(\rho+\mu) = F(\rho) + F(\mu)$ which in particular implies that a.e. on $\{\mu > 0\}$, one has

$$|\nabla\mu|^2 \frac{\rho}{\mu} + |\nabla\rho|^2 \frac{\mu}{\rho} = 2\nabla\mu \cdot \nabla\rho$$

so that

$$\sqrt{\rho}\nabla\sqrt{\mu} = \sqrt{\mu}\nabla\sqrt{\rho} \tag{23}$$

and since $\sqrt{\mu} \in H^1$, $\nabla\sqrt{\mu} = 0$ a.e. on $\{\mu = 0\}$ hence (23) actually holds a.e.; taking the divergence of (23), we get

$$\Delta\sqrt{\mu} = \frac{\sqrt{\mu}}{\sqrt{\rho}}\Delta\sqrt{\rho} = \frac{\phi}{\tau}\sqrt{\mu}$$

and arguing exactly as in step 2, we deduce that μ is $W^{3,p}$ for every $p \in [1, +\infty)$ and everywhere strictly positive. Getting back, to (23) we deduce that the smooth functions $\log\mu$ and $\log\rho$ differ by an additive constant which should be 0 since μ and ρ are probability measures. This proves that $\mu = \rho$ and so that the minimizer of (12) is unique.

Remark 3.3. Note that the full sequence ρ_δ in fact converges to the solution ρ of (12). Let us also remark that the Kantorovich potential ϕ in (13) is defined uniquely (not only up to an additive constant) by the condition

$$\int_{\mathbb{T}^d} \phi\sqrt{\rho} = 0$$

obtained by multiplying (13) by $\sqrt{\rho}$ and integrating.

4. Duality

For $\varphi \in C(\mathbb{T}^d)$, set
$$\varphi^{c_\tau}(y) := \inf_{y\in\mathbb{T}^d} \{\frac{1}{2\tau} \operatorname{dist}^2(x,y) - \varphi(y)\},\ x \in \mathbb{T}^d$$

and
$$V(\varphi) := -\int_{\mathbb{T}^d} \varphi^{c_\tau} \mathrm{d}\rho_0$$

note that V is convex and everywhere finite and continuous on $C(\mathbb{T}^d)$. Moreover, the Kantorovich duality formula can be conveniently expressed in terms of the Legendre transform of V, V^*: $\mathscr{M}(\mathbb{T}^d) \to \mathbb{R} \cup \{+\infty\}$:

$$V^*(\mu) = \begin{cases} \frac{1}{2\tau} W_2^2(\mu, \rho_0) & \text{if } \mu \in \mathscr{P}(\mathbb{T}^d), \\ +\infty & \text{otherwise.} \end{cases}.$$

Consider now the concave maximization problem

$$\sup\Big\{ \int_{\mathbb{T}^d} \Big(\frac{\operatorname{div}\beta - \alpha}{2}\Big)^{c_\tau} \mathrm{d}\rho_0,\ (\alpha,\beta) \in C(\mathbb{T}^d) \times C^1(\mathbb{T}^d, \mathbb{R}^d)\ :\ \alpha + \frac{1}{2}|\beta|^2 \leq 0 \Big\} \tag{24}$$

which can also be written as

$$-\inf_{(\alpha,\beta)\in C(\mathbb{T}^d)\times C^1(\mathbb{T}^d,\mathbb{R}^d)} \Big\{U(\alpha,\beta)+V\Big(\frac{\mathrm{div}\beta-\alpha}{2}\Big)\Big\}$$

where
$$U(\alpha,\beta)=\begin{cases}0 & \text{if } \alpha+\frac{1}{2}|\beta|^2\leq 0 \text{ on } \mathbb{T}^d\\ +\infty & \text{otherwise}\end{cases}$$

whose dual in the sense of Fenchel-Rockafellar see [25] reads:

$$\inf_{\mu\in\mathscr{M}(\mathbb{T}^d)} U^*\Big(\frac{1}{2}(\mu,\nabla\mu)\Big)+V^*(\mu)$$

and since, by (11), we have

$$U^*\Big(\frac{1}{2}(\mu,\nabla\mu)\Big)=\begin{cases}F(\mu) & \text{if } \mu\geq 0 \text{ and } \sqrt{\mu}\in H^1(\mathbb{T}^d)\\ +\infty & \text{otherwise}\end{cases}$$

it follows from the Fenchel-Rockafellar theorem (Theorem 4.1 in [25]) that:

$$\min(12)=\sup(24).$$

Therefore we can say that (12) is the dual of (24). Note that (24) is a slightly unusual optimization problem and it is a priori unclear whether it admits a solution $(\alpha,\beta)\in C(\mathbb{T}^d)\times C^1(\mathbb{T}^d,\mathbb{R}^d)$. But thanks to Theorem 3.1, we can easily find a (smooth) solution of (24):

Proposition 4.1. *Let ρ be the solution of* (12) *then the pair (of $C^{1,\alpha}$ functions)*

$$\alpha:=-\frac{1}{2}|\nabla\log\rho|^2,\ \beta:=\nabla\log\rho \tag{25}$$

is the only solution of (24).

Proof. Note that by construction (α,β) is admissible for (24) and from (13), we have
$$\frac{\phi}{\tau}=\frac{1}{2}\Delta\log\rho+\frac{1}{4}|\nabla\log\rho|^2=\frac{\mathrm{div}\beta-\alpha}{2}$$

where ϕ is a Kantorovich potential between ρ and ρ_0 so that, on the one hand

$$\frac{1}{2\tau}W_2^2(\rho,\rho_0)=\int_{\mathbb{T}^d}\frac{\phi}{\tau}\rho+\int_{\mathbb{T}^d}\Big(\frac{\phi}{\tau}\Big)^{c_\tau}\mathrm{d}\rho_0=\int_{\mathbb{T}^d}\frac{\phi}{\tau}\rho+\int_{\mathbb{T}^d}\Big(\frac{\mathrm{div}\beta-\alpha}{2}\Big)^{c_\tau}\mathrm{d}\rho_0.$$

On the other hand

$$F(\rho)=\frac{1}{4}\int_{\mathbb{T}^d}\frac{|\nabla\rho|^2}{\rho}=\int_{\mathbb{T}^d}\frac{\alpha-\mathrm{div}\beta}{2}\rho=-\int_{\mathbb{T}^d}\frac{\phi}{\tau}\rho.$$

Summing the two equalities above, duality and the fact that ρ solves (12) thus imply

$$\sup(24)=\inf(12)=\frac{1}{2\tau}W_2^2(\rho,\rho_0)+F(\rho)=\int_{\mathbb{T}^d}\Big(\frac{\mathrm{div}\beta-\alpha}{2}\Big)^{c_\tau}\mathrm{d}\rho_0$$

so that (α,β) solves (24).

Now if (a, b) is another solution of (24), one should have

$$F(\rho) = \int_{\mathbb{T}^d} \frac{a\rho + b \cdot \nabla\rho}{2}$$

implying that $a(x)$ and $b(x)$ maximize $a\rho(x) + b \cdot \nabla\rho(x)$ subject to the constraint $a + \frac{1}{2}|b|^2 \leq 0$, but since $\rho(x) > 0$, this constraint should be binding and there is a unique such maximizer which is $(\alpha(x), \beta(x))$ defined in (25). □

5. Numerical solutions by a primal-dual method

The core idea of our numerical scheme is to discretize both the primal (3) and the dual (4) JKO step in space, and then apply the Chambolle-Pock algorithm to optimize in both problems alternatively. It suffices to describe the discretization of the first JKO step, from the datum ρ_0 to the minimizer ρ_1.

5.1. The discretized primal problem

Key to this method is the dual interpretation of the $\mathrm{BB}(r, m)$ functional, see (8)–(9) which is local in space. This local property may be lost after discretisation on a grid because the constraint on (r, m) involves differential operators. In general, special care must be taken to ensure consistency and accuracy, see [47] and [40] for details. In our case, we deal with smooth solutions and positive densities as explained in Theorem 3.1. This, at least heuristically, should enable us to use the same discretisation grid for fluxes and densities and plain centered finite differences, as detailed below.

The torus $\mathbb{T}^d$ is modelled by a box $B = [0, 1]^d$, functions on B extend periodically. For simplicity, we explain the discretization in $d = 1$ space dimensions, the translation to $d > 1$ is straight-forward but notationally cumbersome. We use a cartesian grid with N vertices $x_j := (j + 0.5)\, h$, for $j = 1, \dots, N$, and uniform grid step $h = 1/N$. The centering of the grid points in the cells simplifies the implementation of the periodic boundary conditions. Functions $f : \mathbb{T}^d \to \mathbb{R}$ are discretized by finite sequences $(f_j)_{j=1,\dots,N}$ with $f_j \simeq f(x_j)$. Introduce the L^2 inner product of functions on the grid by

$$\langle f, g\rangle = \frac{1}{N} \sum_j f_j g_j.$$

The central finite difference quotient is denoted by D_h, i.e.,

$$\big(D_h f\big)_j = \frac{f_{j+1} - f_{j-1}}{2h}.$$

Note that D_h is anti self-adjoint with respect to the inner product, i.e., $-D_h^* = D_h$ is also the divergence.

The primal JKO problem (3) is now discretized as follows:

$$\inf_{\rho, m} \left\{ \frac{1}{N} \sum_{j=1}^{N} \frac{m_j^2}{2\,\rho_{0,j}} + \frac{\tau}{N} \sum_{j=1}^{N} \frac{\big(D_h\rho\big)_j^2}{4\,\rho_j} \right\} \tag{26}$$

$$\text{subject to} \quad \rho_j - \rho_{0,j} - \big(D_h^* m\big)_j = 0 \quad \text{for } j = 1, \dots, N. \tag{27}$$

In (26) above, the Fisher information F is simply discretized by finite differences in the second term. The relation between the first term in (26) and the constraint (27) to the dynamical representation (7) of $W_2^2(\rho_0,\rho_1)$ deserves some comment: recall that that in (7), curves $(\rho_s,\mathfrak{m}_s)_{s\in[0,1]}$ depending on a fictitious time $s\in[0,1]$ – unrelated to the physical time t – have been considered to relax the problem. For small $\tau>0$, we expect the initial and terminal densities ρ_0 and ρ_1 to be close, and the momentum $\mathfrak{m}_s\approx\overline{\mathfrak{m}}$ to be almost s-independent. Accordingly, the continuity equation $\partial_s\rho_s+\mathrm{div}\mathfrak{m}_s=0$ should be well-approximated by the stationary equation

$$\rho_1-\rho_0+\mathrm{div}\overline{\mathfrak{m}}=0. \tag{28}$$

For approximation of the s-integral in (7), the denominator ρ_s should be replaced by some average of ρ_0 and ρ_1. The two canonical choices are explicit ($\rho_s\approx\rho_0$ as in [11]) and implicit ($\rho_s\approx\rho_1$ as in [13]). Either choice leads to a linearization of the Wasserstein distance in the form ($i=0$ or 1)

$$\frac{1}{2}W_2^2(\rho_0,\rho_1)\approx\inf_{\overline{\mathfrak{m}}}\left\{\int_{\mathbb{T}^d}\frac{|\overline{\mathfrak{m}}|^2}{2\rho_i}\,:\,-\mathrm{div}\overline{\mathfrak{m}}=\rho_1-\rho_0\right\}. \tag{29}$$

The minimizer is explicitly given by $\overline{\mathfrak{m}}=\rho_i\nabla\phi$, where ϕ solves the linear elliptic equation $-\mathrm{div}(\rho_i\nabla\phi)=\rho_1-\rho_0$ with periodic boundary conditions. In summary, this leads to the explicit ($i=0$) or implicit ($i=1$) approximation

$$W_2^2(\rho_0,\rho_1)\approx\left\|\rho_1-\rho_0\right\|^2_{H^{-1}_{\rho_i}}$$

by a ρ_i-weighted H^{-1}-norm. We refer to Peyre [48] for a detailed comparison between the Wasserstein distance and its weighted H^{-1} linearization. The approximation in (26)-(27) above has been built on the representation (29), in which we have chosen the numerically cheaper explicit form ($i=0$).

Since replacing $W_2^2(\cdot,\rho_0)$ by (the more convenient quadratic) functional $\|\cdot-\rho_0\|^2_{H^{-1}_{\rho_0}}$ introduces an extra source of error in our scheme, we wish to briefly discuss this error at the continuous level i.e. the minimization problem (12). More precisely, given ρ_0 with a smooth and positive density, setting

$$L_{\rho_0}:=\|\cdot-\rho_0\|^2_{H^{-1}_{\rho_0}},$$

consider

$$\rho_\tau=\mathrm{argmin}\left\{\tau F+\frac{1}{2}W_2^2(\cdot,\rho_0)\right\},\ \alpha_\tau=\mathrm{argmin}\left\{\tau F+\frac{1}{2}L_{\rho_0}\right\}.$$

Arguing slightly heuristically as in the end of Chapter 7 from [50] (see also [48] for more details), when μ is close to ρ_0 and has a positive and smooth density, there holds

$$W_2^2(\mu,\rho_0)=L_{\rho_0}(\mu)+o(L_{\rho_0}(\mu)). \tag{30}$$

Since α_τ is smooth and positive, this entails:

$$\frac{1}{2}W_2^2(\rho_\tau,\rho_0)=\frac{1}{2}L_{\rho_0}(\rho_\tau)+o(L_{\rho_0}(\rho_\tau))\leq\tau(F(\rho_0)-F(\rho_\tau))=O(\tau), \tag{31}$$

and by the very definition of α_τ, we also have

$$\frac{1}{2}L_{\rho_0}(\alpha_\tau)\leq\tau(F(\rho_0)-F(\alpha_\tau))=O(\tau). \tag{32}$$

Using the fact that α_τ is a critical point of the functional $\tau F + \frac{1}{2}L_{\rho_0}$ which is more convex than the quadratic term $\frac{1}{2}L_{\rho_0}$, we get

$$\begin{aligned}
&\frac{1}{2}\|\rho_\tau - \alpha_\tau\|^2_{H^{-1}_{\rho_0}} \leq \frac{1}{2}L_{\rho_0}(\rho_\tau) + \tau F(\rho_\tau) - \frac{1}{2}L_{\rho_0}(\alpha_\tau) - \tau F(\alpha_\tau)\\
&\leq \frac{1}{2}W_2^2(\rho_\tau, \rho_0) + \tau F(\rho_\tau) - \frac{1}{2}W_2^2(\alpha_\tau, \rho_0) - \tau F(\alpha_\tau) + o(L_{\rho_0}(\rho_\tau) + L_{\rho_0}(\alpha_\tau))\\
&\leq o(\tau)
\end{aligned}$$

where we used (31)–(32) in the second line and the construction of ρ_τ in the last line. We thus have an error bound of the form $\|\rho_\tau - \alpha_\tau\|_{H^{-1}_{\rho_0}} = o(\tau^{\frac{1}{2}})$.

5.2. The discretized dual problem

Somehow mimicking the continuous duality formulation, using the fact that the (discretized) linearized Wasserstein term can be written in dual form via the support function of the parabola K as in (9), we can reformulate (26)–(27) in inf-sup form

$$\inf_{\rho,m} \sum_{j=1}^N \frac{m_j^2}{2\,\rho_{0,j}} + \sup_{\phi,(\alpha,\beta)\in K} \Big\{ \langle \phi, \rho - \rho_0 - D_h^*(m)\rangle + \frac{\tau}{2}\langle \alpha, \rho\rangle + \frac{\tau}{2}\langle \beta, D_h(\rho)\rangle \Big\} \tag{33}$$

by standard arguments (see chapter VI in [25]) the above Lagrangian has a saddle point and the dual is obtained by switching the inf and the sup. Doing so, we obtain that the saddle point satisfies

$$m = \rho_0 D_h \phi,\ \phi + \frac{\tau}{2}(\alpha + D_h^* \beta) = 0$$

from which we can eliminate the variable $\alpha = -\frac{2\phi}{\tau} - D_h^*\beta$ so that (ϕ, β) solves the dual of (26)-(27) which can be written as

$$\inf_{(\phi,\beta)} \Big\{ \frac{1}{2N}\sum_{j=1}^N \rho_{0,j}\big(D_h\phi\big)_j^2 + \langle \phi, \rho_0\rangle \ :\ (-\frac{2\phi}{\tau} - D_h^*\beta, \beta) \in K \Big\} \tag{34}$$

where of course, we have changed the sign in the dual to have a convex minimization problem instead of a concave maximization one.

As we shall see in the next paragraph, problem (34) is amenable to the Chambolle-Pock algorithm, and finding the optimal ϕ we can of course recover the optimal ρ (nonnegative by construction since $\sigma_K(\rho, m) = +\infty$ if not) by

$$\rho = \rho_0 + D_h^*(\rho_0 D_h \phi).$$

5.3. Solution by the Chambolle-Pock algorithm

Given two lsc convex functions Φ: $\mathbb{R}^p \to \mathbb{R} \cup \{+\infty\}$, $\Psi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ and Λ an $n \times p$ matrix, consider the convex minimization

$$\inf_{z\in\mathbb{R}^p}\{\Phi(z) + \Psi(\Lambda z)\} = \inf_{z\in\mathbb{R}^p}\Big\{\Phi(z) + \sup_{q\in\mathbb{R}^n}\{q\cdot\Lambda z - \Psi^*(q)\}\Big\}. \tag{35}$$

Recalling that for a convex lsc function G: $\mathbb{R}^p \to \mathbb{R} \cup \{+\infty\}$, the proximal operator of G is defined by

$$\operatorname{prox}_G(x) = (\operatorname{id} + \partial G)^{-1}(x) := \operatorname*{argmin}_{y \in \mathbb{R}^p} \{\frac{1}{2}|x-y|^2 + G(y)\}, \ \forall x \in \mathbb{R}^p$$

and that G is called simple whenever prox_G (or $\operatorname{prox}_{\sigma G}$) can be computed in closed form. By Moreau's identity (see [3]):

$$\operatorname{prox}_{G^*} = \operatorname{id} - \operatorname{prox}_G$$

we see that G^* is simple as soon as G is. Note also that if G is the characteristic function of a closed convex set C, prox_G is the projection onto C, hence, if projecting onto C is closed form, both G and its Legendre transform $G^* = \sigma_C$ (the support function of C) are simple.

The Chambolle-Pock primal-dual algorithm consists in iterating the proximal steps:

$$q^{t+1} = \operatorname{prox}_{\sigma\Psi^*}(q^t + \sigma\Lambda x^t) \tag{36}$$

$$z^{t+1} = \operatorname{prox}_{\delta\Phi}(z^t - \delta\Lambda^* q^{t+1}) \tag{37}$$

and the extrapolation step
$$x^{t+1} = 2z^{t+1} - z^t. \tag{38}$$

Chambolle and Pock proved in [19], that, provided:

- there exists a saddle point for (35) (i.e. a pair (z, q) such that $q \in \partial\Psi(\Lambda z)$ and $-\Lambda^* q \in \partial\Phi(z)$),
- the (positive) steps σ and δ are chosen such that

$$\sigma\delta\|\Lambda\|_{\mathrm{op}}^2 < 1, \tag{39}$$

then, the Chambolle-Pock iterates (z^t, q^t) converge to a saddle point (so that the first component solves (35) and the second solves its dual). Chambolle-Pock certainly is a good choice for solving (35) if Φ and Ψ are nonsmooth but simple (note that contrarily to ADMM we never have to project on the range of Λ but just to compute Λx^t and $\Lambda^* q^{t+1}$).

Let us now consider (34) and write it in the standard form (35), setting

$$z = (\phi, \beta), \quad \text{and} \quad \Lambda z = (-\frac{2\phi}{\tau} - D_h^* \beta, \beta). \tag{40}$$

Remark that $\|\Lambda\|_{\mathrm{op}} \sim \max(\tau^{-1}, h^{-1})$ which depends directly on the time and space discretization steps, how these steps and σ and δ are chosen in practice will be discussed in paragraph 5.4. Then (34) corresponds to

$$\Phi(z) = \frac{1}{2N} \sum_{j=1}^{N} \rho_{0,j} \left(D_h\phi\right)_j^2 + \langle \phi, \rho_0 \rangle$$

and
$$\Psi(\alpha, \beta) = \begin{cases} 0 & \text{if } (\alpha_j, \beta_j) \in K \text{ for } j = 1, \dots, N \\ +\infty & \text{otherwise.} \end{cases}$$

Observe first that Ψ is simple since the projection onto K which can be performed on each grid point is almost explicit (see [4] and [47] for details).

As for the weighted discretized Dirichlet energy Φ, it is also simple since computing its proximal operator amounts to solve a linear system discretizing a linear elliptic equation. More precisely $\mathrm{prox}_{\delta\Phi}(\phi_0, \beta_0) = (\phi, \beta_0)$ where ϕ solves

$$\phi + \delta D_h^*\big(\rho_0\, D_h\phi\big) = \phi_0 - \delta\rho_0.$$

This shows the feasibility of the Chambolle-Pock algorithm for (34) which is illustrated in the next paragraph. Note that the convergence is ensured but can be quite slow, see Figure 1 for convergence curves and a discussion associated with the test cases of Section 5.4.

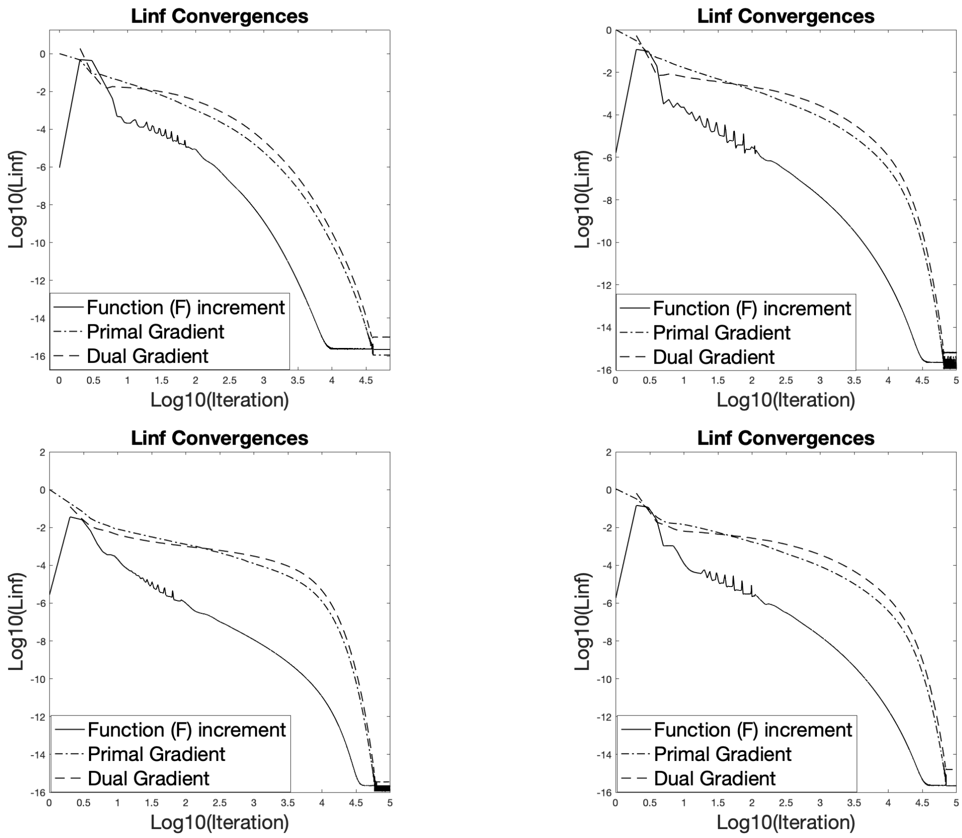


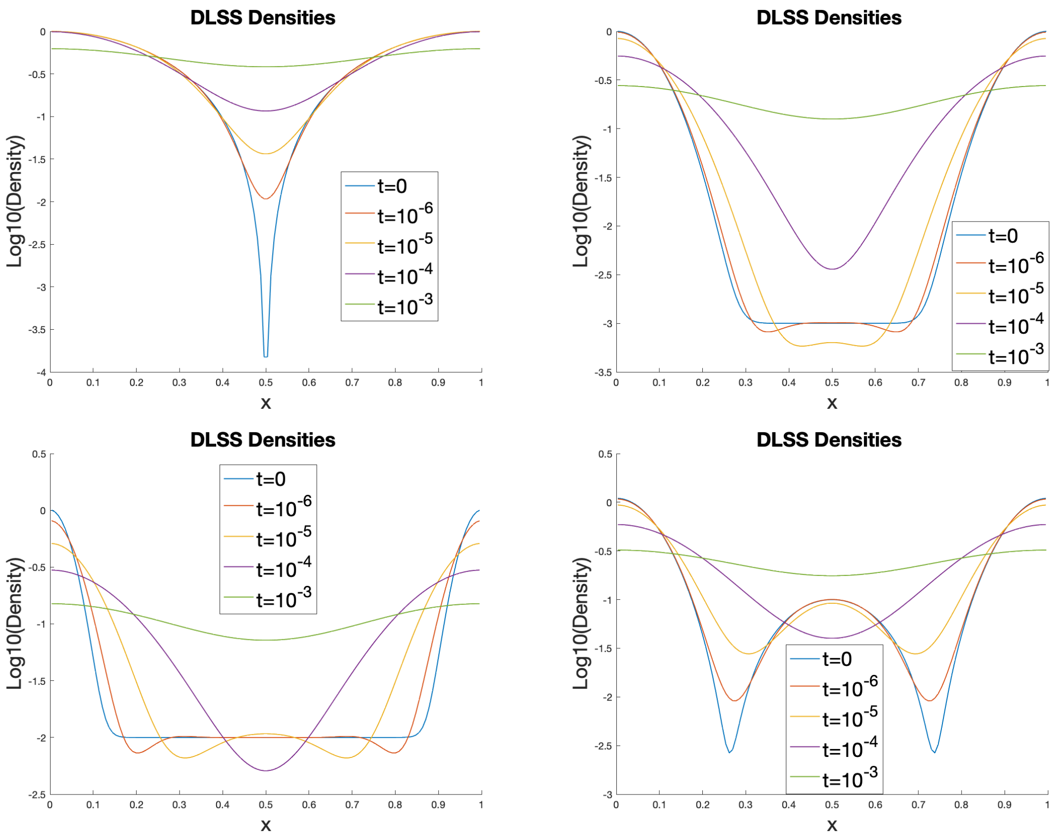
Figure 1: Convergence for the first KO step starting with (41). Test 1 to 4, left to right and top to bottom. In $\|.\|_\infty$ norm we show the iteration increment on F, and also the primal and dual gradient error respectively $\|\Lambda^* q + \partial\Phi(z)\|_\infty$ and $\|\Lambda z - \partial\Psi^*(q)\|_\infty$.

5.4. Simulations

The method described above is used to perform simulations in $d = 1$ and periodic boundary conditions. We use the following set of test cases :

$$\begin{aligned}
&\text{Test 1:} \quad \rho_0(x) = \cos^2(\pi x).\\
&\text{Test 2:} \quad \rho_0(x) = 10^{-3} + \cos^{16}(\pi x).\\
&\text{Test 3:} \quad \rho_0(x) = 10^{-2} + \cos^{64}(\pi x).\\
&\text{Test 4:} \quad \rho_0(x) = 10^{-1} + \cos^{16}(\pi x) - \sin^2(2\,\pi\, x).
\end{aligned} \tag{41}$$

Test cases 1 and 2 were treated in [8] providing reference results, the proposed test cases 3 and 4 are similar. Simulations show (Figure 2) a fast diffusion towards a constant equilibrium (there is no forcing potential). The results are consistent with Figure 1 on page 15 in [8].



Figur 2: DLSS with initialisation (41), Test 1 to 4, left to right and top to bottom.

Choice of numerical parameters: We have been using $N = 128$ grid points in space (i.e. $1/h = N = 128$). The DLSS Finite Difference discretisation approach in [8] uses a time discretization τ of the order of h^4 (the authors of [8] take $1/h = N = 100$ and $\tau = 10^{-8}$). We observed *experimentally* that our method gives consistent results using exponentially increasing time steps. We take $h_0 = 10^{-7}$ and $h_k = 10^k\, h_0$. This choice a a strong impact on the convergence (at each time step) of the Chambolle Pock Algorithm. It depends on the norm of the operator Λ which is of the order $\|\Lambda\|_{\text{op}} \sim \max(\tau^{-1}, h^{-1})$ (see (40) in section 5.3). We therefore expect that the convergence will be slow at the begining and improving as the the time step increases. This is what we observe in practice, the first iteration generally needs 10^5 iterations to converge to machine precision, see Figure 2 and as time t increases, the last JKO steps are computed with “only” 10^3 Chambolle-Pock iterations (not represented). Finally, for the Chambolle-Pock steps, we have used $\sigma = 1/2$ and $\delta = 0.99/(\sigma\, \|\Lambda\|^2_{\text{op}})$ to comply with the convergence condition (39).

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