

A Computational Fluid Mechanics solution to the Monge-Kantorovich mass transfer problem.

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Abstract

The L^2 Monge-Kantorovich mass transfer problem [31] is reset in a Fluid Mechanics framework and numerically solved by an augmented Lagrangian method.

1 Introduction

The first mass transfer problem was considered by Monge in 1781 in his “*mémoire sur la théorie des déblais et des remblais*”, a Civil Engineering problem where parcels of materials have to be displaced from one site to another one with minimal transportation cost. A modern treatment of this problem has been initiated by Kantorovich in 1942 (cf. [23] for the english version), leading to the so-called Monge-Kantorovich problem which has received a considerable interest in the recent years, with a wide range of potential applications and extensions. A recent comprehensive review can be found in the new books by Rachev and Rüschendorf [31], the lecture notes by Evans [19] and the review paper by McCann and Gangbo [21].

The framework of the Monge-Kantorovich problem is as follows. Two density functions $\rho_0(x) \geq 0$ and $\rho_T(x) \geq 0$ of $x \in \mathbb{R}^d$, that we assume to be bounded with total mass one

$$\int_{\mathbb{R}^d} \rho_0(x) dx = \int_{\mathbb{R}^d} \rho_T(x) dx = 1, \quad (1)$$

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are given. We say that a map M from \mathbb{R}^d to \mathbb{R}^d realizes the transfer of ρ_0 to ρ_T if, for all bounded subset A of \mathbb{R}^d ,

$$\int_{x \in A} \rho_T(x) dx = \int_{M(x) \in A} \rho_0(x) dx. \quad (2)$$

If M is a smooth one-to-one map, (2) just means

$$\det(\nabla M(x)) \rho_T(M(x)) = \rho_0(x), \quad (3)$$

where \det denotes determinants for $d \times d$ matrices, which is often referred as the ‘‘jacobian equation’’. The ‘‘jacobian problem’’, consisting in finding such a map M , given ρ_0 and ρ_T , has been solved by Moser [27] and Dacorogna and Moser [17] with two different constructive methods that can both lead to effective numerical algorithms (see [7] for applications in Chemistry). Clearly the jacobian problem is underdetermined and it is natural to select among the maps satisfying (2) those which are optimal in a suitable sense. One way is to introduce the so-called L^p Kantorovich (or Wasserstein) distance between ρ_0 and ρ_T defined by :

$$d_p(\rho_0, \rho_T)^p = \inf_M \int |M(x) - x|^p \rho_0(x) dx, \quad (4)$$

where $p \geq 1$ is fixed, $|\cdot|$ denotes the euclidean norm in \mathbb{R}^d and the infimum is taken among all map M transporting ρ_0 to ρ_T . Whenever the infimum is achieved by some map M , we say that M is an optimal transfer and solves the L^p Monge-Kantorovich problem (MKP).

Two exponents p are particularly interesting. The original Monge transfer problem corresponds to $p = 1$ and has been studied by Sudakov [35] (see [19] and the relationship with sandpile models). The case $p = 2$, the only one addressed in the present paper, has remarkable properties and, as we shall see, is directly related to Continuum Mechanics. Let us just briefly mention the theoretical importance of the L^2 MKP in many different fields such as Probability Theory and Statistics [31], Functional Analysis [3], Kinetic Theory (where the L^2 Kantorovich distance is closely related to the homogeneous Boltzmann equation of maxwellian molecules and the Fokker-Planck equation [36], [22]), Atmospheric Sciences (where the construction of the semi-geostrophic model by Cullen and Purser is based on a variant of the L^2 MKP [16], [6]), Astrophysics [26], Porous media equations, Hele-Shaw equations (with the new approach introduced by Otto for dissipative PDEs viewed as gradient flows with respect to the L^2 Kantorovich metric [28],[29]). From a more computational point of view, the Kantorovich distance is a valuable quantitative information to compare two different density functions, which may be used in various fields of applications, such as shape recognition in image processing, computer vision and signal treatment, data assimilation in meteorology and oceanography, quantum chemistry etc.

Let us recall a basic theoretical result on the L^2 MKP ([24], [8], [10], see also [31], [21],[19]) : there is a unique optimal transfer M characterized as the unique map transferring ρ_0 to ρ_T which can be written as the gradient of some convex function Ψ ,

$$M(x) = \nabla \Psi(x). \quad (5)$$

Moreover, because of (2), Ψ is a solution (in a suitable weak sense) of the Monge-Ampère equation

$$\det(H\Psi(x))\rho_T(\nabla\Psi(x)) = \rho_0(x), \quad (6)$$

(where $H\Psi$ is the Hessian matrix of Ψ). Moreover Ψ inherits the smoothness of ρ_0 and ρ_T under additional geometrical conditions, as shown by Caffarelli [13].

It follows from this theoretical result that a natural computational solution of the L^2 MKP is the numerical resolution of the Monge-Ampère equation (6). Unfortunately, this fully non-linear second-order elliptic equation has not received much attention from numerical analysts and, to the best of our knowledge, there is no efficient finite-difference or finite-element methods, comparable to those developed for linear second-order elliptic equations (such as fast Poisson solvers, multigrid methods, preconditioned conjugate gradient methods,...). In addition, the mass transfer problem involving (6) is not a standard boundary value problems even when ρ_0 vanishes along a smooth subset of \mathbb{R}^d . A geometrical method has been designed at the UK met'office by Cullen and Purser [16], [14], in view of the numerical resolution of the semi-geostrophic equations, using an approach similar to Pogorelov's constructive proof of existence for the Monge-Ampère equation [30]. A similar method is used in [25] for the design of antennas. A domain decomposition method for problem (6) has also been proposed in [4] and used for a simplified semi-geostrophic model in [5].

In the present paper, we introduce an alternative numerical method for the L^2 MKP, avoiding the direct solution of (6), based on a resetting of the mass transfer problem into a Continuum Mechanics framework. To do that, we fix a time interval $[0, T]$ and consider all possible smooth enough, time-dependent, density et velocity fields, $\rho(t, x) \geq 0$, $v(t, x) \in \mathbb{R}^d$, subject to the continuity equation

$$\partial_t \rho + \nabla \cdot (\rho v) = 0 \quad (7)$$

for $0 < t < T$ and $x \in \mathbb{R}^d$, and the initial and final conditions

$$\rho(0, \cdot) = \rho_0, \quad \rho(T, \cdot) = \rho_T. \quad (8)$$

Then, we will observe

Proposition 1.1 *The square of the L^2 Kantorovich distance is equal to the infimum of*

$$T \int_{\mathbb{R}^d} \int_0^T \rho(t, x) |v(t, x)|^2 dx dt, \quad (9)$$

among all (ρ, v) satisfying (7) and (8).

The formal optimality conditions of this space-time minimization problem turn out to be

$$v(t, x) = \nabla \psi(t, x), \quad (10)$$

where the potential ϕ is the Lagrange multiplier of constraints (7), (8), and the Hamilton-Jacobi equation

$$\partial_t \phi + \frac{1}{2} |\nabla \phi|^2 = 0. \quad (11)$$

In terms of Fluid Mechanics, this says that the optimal solution is simply given by a pressureless potential flow.

Let us point out that a Continuum Mechanics formulation was already implicitly contained in the original problem addressed by Monge : “le problème des remblais et des déblais”. Eliminating the time variable was just a clever way of reducing the dimension of the problem. However, from a computational point of view, reintroducing the time variable allows to solve a convex (although not quadratic) space-time minimization problem in the density and momentum variables, namely ρ and $m = \rho v$, with linear constraints, namely (7) and (8), instead of the original one, defined by (4), which is a quadratic space minimization problem in M , with a non-linear, non-convex and highly degenerate constraint (2). This is in our opinion a considerable advantage, in spite of the addition of the extra (but not artificial) time variable. In addition, the Continuum Mechanics formulation, provides a natural time interpolant $\rho(t, x)$ of the data ρ_0 and ρ_T and a velocity field $v(t, x)$ which moves ρ_0 toward ρ_T , which may be useful for practical applications, in particular for computational vision. (Notice that our approach is somewhat related to recent techniques used in computer vision based on elastic motions, such as the geometric approach of [38].)

The new space-time minimization problem will be solved as a saddle-point problem for a suitable Lagrangian. To do that, a space-time dependent Lagrange multiplier $\phi(t, x)$ will be used for the linear constraints (7) and (8), the integrand of (9) will be written as a Legendre transform

$$\frac{1}{2} \rho |v|^2 = \sup \{ a \rho + b \cdot \rho v ; a + \frac{1}{2} |b|^2 \leq 0 \}, \quad (12)$$

and the corresponding space-time dependent dual variables $a(t, x) \in \mathbb{R}$ and $b(t, x) \in \mathbb{R}^d$ will also be used. In the saddle-point problem, the original unknowns, namely the density ρ and the momentum $m = \rho v$, become the Lagrange

multipliers for the new constraint

$$a - \partial_t \phi = 0, \quad b - \nabla \phi = 0. \quad (13)$$

Following a classical technique of Computational Continuum Mechanics, the so-called augmented Lagrangian method [20], the Lagrangian will be augmented by the squared L^2 norm of the new constraint (13) and Uzawa's gradient method will be used, corresponding to the so-called ALG2 algorithm of [20]. Because of the use of the dual variables (a, b) , each gradient step amounts to solve three elementary computational problems : Step 1 is a space-time constant-coefficient Laplace equation in ϕ with homogeneous Neumann boundary conditions in space and non-homogeneous Neumann conditions in time, for which fast solvers can be used, Step 2 is a *pointwise* minimization in a and b , which amounts to minimize at each space-time grid point a convex function of one real variable, Step 3 is a trivial updating of the main unknowns ρ and m . So our method is very easy to code and the computational cost of each iteration of the Uzawa method is nearly optimal. Numerical examples will be shown, in two space dimensions, on the unit square with periodic boundary conditions. A non-trivial example will be the transfer of two shifted periodic arrays of gaussian densities. Our method will be able to pick up the change of topology of the contour lines due to the particular geometry of the periodic square.

Let us outline the content of the paper : In section 2, we make a short review of the L^2 MKP, including some elementary examples and possible applications and extensions. In section 3, we justify Proposition 1.1. In section 4, we describe the algorithm. Finally, numerical examples will be provided in section 5.

2 Examples of MKP and generalizations.

The assignment problem.

The data ρ_0 and ρ_T can be much more general than bounded functions and probability measures can also be considered [31]. In particular, we can consider weighted sums of delta functions, such as

$$\rho_0(x) = \frac{1}{N} \sum_{i=1, N} \delta(x - x_i), \quad \rho_T(x) = \frac{1}{N} \sum_{i=1, N} \delta(x - y_i), \quad (14)$$

where the $2N$ points $x_1 \in \mathbb{R}^d, \dots, x_N \in \mathbb{R}^d, y_1 \in \mathbb{R}^d, \dots, y_N \in \mathbb{R}^d$ are given. Then the L^2 Kantorovich distance is simply

$$d_2(\rho_0, \rho_T)^2 = \inf_{\sigma} \sum_{i=1, N} |y_i - x_{\sigma(i)}|^2, \quad (15)$$

where the infimum is performed over all permutations $i \rightarrow \sigma(i)$. This is a particular case of one of the most basic (and polynomial) problems in Combinatorial Optimization, the linear assignment problem [3], which has the general structure

$$\inf_{\sigma} \sum_{i=1, N} c(i, \sigma(i)), \quad (16)$$

where $(c(i, j), i, j = 1, N)$ is a given “cost” matrix. Here

$$c(i, j) = |x_i - y_j|^2. \quad (17)$$

This problem can be solved as a linear programming problem, following Kantorovich’ approach [23], after noticing that (16) can be written

$$\inf_{\mu} \sum_{i, j=1, N} c_{ij} \mu_{ij}, \quad (18)$$

where $c_{ij} = |x_i - y_j|^2$ is the so-called cost matrix and μ denotes any $N \times N$ matrix with nonnegative entries, such that the sum of all columns and rows is always equal to one. (These matrices, called doubly-stochastic matrices, define a convex set the extreme points of which exactly are the permutation matrices). There are nearly optimal algorithms for general cost matrices, with a computational cost of order $O(N^2 \log N)$, such as Balinski’s algorithm [2]. However, to the best of our knowledge, there is no optimal algorithm for the special structure (17).

The MKP on the real line.

In the one dimensional case $d = 1$, the convexity of potential Ψ just means that the optimal mass transfer $x \rightarrow M(x)$ is a non-decreasing function. Thus, M is entirely determined by (2) through

$$\int_{y < M(x)} \rho_T(y) dy = \int_{y < x} \rho_0(y) dy, \quad \forall x \in \mathbb{R}, \quad (19)$$

which can be easily solved numerically. As a matter of fact, in this case, the linear assignment problem (16) with cost (17) is equivalent to sorting the points x_i and y_i in increasing order.

Dilated and translated densities.

Let us assume that ρ_T is compactly supported in \mathbb{R}^d and obtained from ρ_0 through a dilation and a translation

$$\rho_T(x) = r^d \rho(r(x - c)), \quad (20)$$

for some $r > 0$ and $c \in \mathbb{R}^d$, and ρ_0 is normalized so that

$$\int x \rho_0(x) dx = 0, \quad \int |x|^2 \rho_0(x) dx = 1. \quad (21)$$

Then it can be checked that the optimal transfer is simply given by $M(x) = r^{-1}x + c$, which yields

$$d_2(\rho_0, \rho_T)^2 = (1 - r^{-1})^2 + |c|^2. \quad (22)$$

Extension to more complex Fluid Mechanics models.

As already mentioned, the formal optimality condition for ρ and v correspond to the evolution of a potential pressureless flow, a very crude model in Fluid Mechanics. More interesting models for use in Meteorology and Oceanography can be related to the MKP. In is well known, for instance, that the Euler equations for an ideal incompressible fluid

$$(\partial_t + v \cdot \nabla)v = -\nabla p, \quad \nabla \cdot v = 0, \quad (23)$$

in which $p(t, x)$ is the pressure field, obey a least action principle [1]. The Euler equations have been studied as a space-time minimization problem by Shnirelman [33], [34] and Brenier [9], [12], and numerically in [32]. In [12], a generalized MKP is used to characterize the limits of the minimizing sequences, where the density and velocity fields depend on an additional variable $a \in [0, 1]$ (which correspond to a Lagrangian label). These are denoted by $\rho_0(x, a)$, $\rho_T(x, a)$, for the data and $\rho(t, x, a)$, $v(t, x, a)$ for the unknowns. Constraints (8), (7) are enforced for each value of a . The problem is now to minimize

$$T \int_{\mathbb{R}^d} \int_0^T \int_0^1 \rho(t, x, a) |v(t, x, a)|^2 dx dt da. \quad (24)$$

The new feature of this problem lies in the additional constraint on the densities at each point (t, x) :

$$\int_0^1 \rho(t, x, a) da = 1. \quad (25)$$

This equation comes from the incompressibility constraint and pressure $p(t, x)$ is indeed the associated Lagrange multiplier.

In the simpler case when a is a discrete variable and da the counting measure, we recover the homogenized vortex sheet model discussed in [11].

The numerical method introduced in the present paper can in principle be directly generalized to such problems, in which time cannot be eliminated.

Interpolation of the L^2 and the Kantorovich distances

When two densities ρ_0 and ρ_T must be compared, it is very natural to use the L^2 Kantorovich distance. However, sometimes, the regular L^2 distance :

$$d_{L^2}(\rho_0, \rho_T)^2 = \int |\rho_0(x) - \rho_T(x)|^2 dx \quad (26)$$

may be more appropriate. Both situations occur in the case of data assimilation for meteorological forecasting (cf. M.J.Cullen, private communication, see also [18]). A combination of these metrics may therefore be desired for practical applications. A nice interpolation of the L^2 and Kantorovich distances between ρ_0 and ρ_T , for $\theta \in [0, 1]$, is naturally provided by the time continuous formulation, where (8), (7) are unchanged and the cost functional is replaced by :

$$\int_{\mathbb{R}^d} \int_0^1 [(1 - \theta)\rho(t, x)|v(t, x)|^2 + \theta(\partial_t \rho(t, x))^2] dx dt \quad (27)$$

(here T is normalized to 1). Indeed, $\theta = 0$ and $\theta = 1$ respectively give back the L^2 Kantorovich distance and the regular L^2 distance. A remarkable feature of this problem is its formal optimality condition

$$(1 - \theta)(\partial_t + v \cdot \nabla)v + \theta \partial_{tt} \nabla \rho = 0, \quad (28)$$

which is nothing but the Boussinesq equation without gravity term [37].

3 Justification of the Fluid Mechanics formulation of the MKP.

The proof of Proposition 1.1 is easily obtained by using Lagrangian coordinates. We assume ρ_0 and ρ_T to be compactly supported in \mathbb{R}^d and bounded. Let us consider (sufficiently smooth) fields ρ and v satisfying (7), (8). We use Lagrangian coordinates and define $X(t, x)$ by :

$$X(0, x) = x, \quad \partial_t X(t, x) = v(t, X(t, x)), \quad (29)$$

so that, for all test functions f ,

$$\int f(t, x)\rho(t, x) dx dt = \int f(t, X(t, x))\rho_0(x) dx dt, \quad (30)$$

$$\int f(t, x)\rho(t, x)v(t, x) dx dt = \int \partial_t X(t, x) f(t, X(t, x))\rho_0(x) dx dt. \quad (31)$$

Notice first that (8) and (30) imply that $M(x) = X(T, x)$ satisfies condition (2), just as the optimal map $\nabla \Psi(x)$ does. Next, we observe that

$$T \int_{\mathbb{R}^d} \int_0^T \rho(t, x)|v(t, x)|^2 dx dt = T \int_{\mathbb{R}^d} \int_0^T \rho_0(x)|v(t, X(t, x))|^2 dx dt$$

(by (30))

$$= T \int_{\mathbb{R}^d} \int_0^T \rho_0(x) |\partial_t X(t, x)|^2 dx dt$$

(by (29))

$$\geq \int_{\mathbb{R}^d} \rho_0(x) |X(T, x) - X(0, x)|^2 dx$$

(by Jensen's inequality)

$$= \int_{\mathbb{R}^d} \rho_0(x) |X(T, x) - x|^2 dx$$

(by (29) again)

$$\geq \int_{\mathbb{R}^d} \rho_0(x) |\nabla \Psi(x) - x|^2 dx$$

(because both $X(T, x)$ and $\nabla \Psi(x)$ satisfy condition (2), as already mentioned, and $\nabla \Psi$ is the optimal map).

Thus, the optimal choice of $X(t, x)$ is given by

$$X(t, x) = x + \frac{t}{T} (\nabla \Psi(x) - x), \quad (32)$$

which corresponds to the pair (ρ, v) defined by :

$$\int f(t, x) \rho(t, x) dt dx = \int f(t, x + t \frac{\nabla \Psi(x) - x}{T}) \rho_0(x) dt dx, \quad (33)$$

$$\int f(t, x) \rho(t, x) v(t, x) dt dx = \quad (34)$$

$$\int \frac{\nabla \Psi(x) - x}{T} f(t, x + t \frac{\nabla \Psi(x) - x}{T}) \rho_0(x) dt dx,$$

for all test functions f . This completes the proof of Proposition 1.1.

4 The numerical method.

The computational domain is the periodic box $D = \mathbb{R}^d / \mathbb{Z}^d$ and the following notations will be used :

- ∇_x is the spatial gradient,
- $\nabla_{t,x} = \{\partial_t, \nabla_x\}$ is the time-space gradient,
- $\Delta_{t,x} = \partial_t^2 + \Delta_x$ is the time-space Laplacian,
- for two vectors in $\mathbb{R} \times \mathbb{R}^d$, a, b and a', b' , $\{a, b\} \cdot \{a', b'\} = aa' + b \cdot b'$ denotes the inner product.

The L^2 MKP can be written as a saddle-point problem by introducing a space-time dependent Lagrange multiplier $\phi(t, x)$ for constraints (7) and (8). The Lagrangian is given by :

$$L(\phi, \rho, m) = \int_0^T \int_D \left[\frac{|m|^2}{2\rho} - \partial_t \phi \rho - \nabla_x \phi \cdot m \right] - \int_D [\phi(0, \cdot) \rho_0 - \phi(T, \cdot) \rho_T], \quad (35)$$

where the terms involving ϕ come from the integration by part of (7) using boundary conditions (8).

Given initial and final densities ρ_0 and ρ_T , the L^2 MKP is equivalent to the saddle-point problem :

$$\inf_{\rho, m} \sup_{\phi} L(\phi, \rho, m). \quad (36)$$

The (formal) optimality conditions for this problem are :

$$\begin{cases} \partial_t \phi + \frac{|m|^2}{2\rho} = 0, & \frac{m}{\rho} = \nabla_x \phi \\ \partial_t \rho + \nabla_x \cdot m = 0, & \rho(0, \cdot) = \rho_0, \quad \rho(T, \cdot) = \rho_T. \end{cases} \quad (37)$$

Notice that m can be eliminated and the equations of a pressureless potential flow, namely (10), (7), (11) are then recovered.

A new Lagrangian.

In this subsection we build a new Lagrangian for which the methods of [20] can be applied very easily. Let us first observe that, for positive ρ , we have, pointwise in time and space,

$$\frac{|m(t, x)|^2}{2\rho(t, x)} = \sup_{\{a, b\} \in K} [a(t, x) \rho(t, x) + b(t, x) \cdot m(t, x)] \quad (38)$$

where

$$K = \{ \{a, b\} : \mathbb{R} \times \mathbb{R}^d \rightarrow \mathbb{R} \times \mathbb{R}^d, \text{ s. t. } a + \frac{|b|^2}{2} \leq 0 \text{ pointwise} \}. \quad (39)$$

Notice that the left-hand side of (38) becomes infinite whenever ρ vanishes or ρ is positive and m vanishes. Let us introduce the following variables and notations :

$$\mu = \{\rho, m\} \quad q = \{a, b\}, \quad \langle \mu, q \rangle = \int_0^T \int_D \mu \cdot q, \quad (40)$$

$$F(q) = 0 \text{ if } q \in K, \quad +\infty \text{ else,} \quad G(\phi) = \int_D [\phi(0, \cdot) \rho_0 - \phi(T, \cdot) \rho_T]. \quad (41)$$

We now claim that we can write problem (36) as :

$$\sup_{\mu} \inf_{\phi, q} [F(q) + G(\phi) + \langle \mu, \nabla_{t,x} \phi - q \rangle]. \quad (42)$$

To prove this formula, we first use (38) in (35). With the new notations, we get for (36)

$$-\inf_{\rho, m} \sup_{\phi} L(\phi, \rho, m) = \sup_{\rho, m} \inf_{\phi} [G(\phi) + \int_0^T \int_D (\mu \cdot \nabla_{t,x} \phi - \sup_{q \in K} \mu \cdot q)]. \quad (43)$$

Here $q = \{a, b\}$ is meant to be the dual variable of $\mu = \{\rho, m\}$. We now remark that :

$$\int_0^T \int_D \sup_{q \in K} \mu \cdot q = \sup_q [-F(q) + \int_0^T \int_D \mu \cdot q]$$

and we finally get (42) from (43), as claimed.

Such Lagrangian formulations are used in [20] for solving problems of the form

$$\min_v \{F(Bv) + G(v)\},$$

where F, G are convex functionals and B is a linear operator. In order to fully comply with the hypothesis on F, G , and B used in [20], we lack coercivity on F . A simple way to fix this problem is to replace F by the perturbed function F_{ϵ_1} :

$$F_{\epsilon_1}(q) = F(q) + \epsilon_1 \langle q, q \rangle.$$

However, in practice, we obtain fully satisfactory results just with $\epsilon_1 = 0$.

The augmented Lagrangian.

In the new saddle-point problem (42), we can now consider $\mu = \{\rho, m\}$ as the Lagrange multiplier of a new constraint acting on ϕ , namely

$$\nabla_{t,x} \phi - q. \quad (44)$$

(Notice that ϕ was the Lagrange multiplier of constraint (7) in the original saddle-point problem (36).)

Thus, we define the ‘‘augmented’’ Lagrangian :

$$L_r(\phi, q, \mu) = F(q) + G(\phi) + \langle \mu, \nabla_{t,x} \phi - q \rangle + \frac{r}{2} \langle \nabla_{t,x} \phi - q, \nabla_{t,x} \phi - q \rangle \quad (45)$$

where r is a positive parameter and the corresponding saddle-point problem

$$\sup_{\mu} \inf_{\phi, q} L_r(\phi, q, \mu), \quad (46)$$

which clearly has the same solutions as (36).

The algorithm.

A simple algorithm of [20], called ALG2, based on relaxations of the Uzawa algorithm is now used to solve the problem. We get a three step iterative method which constructs a sequence (ϕ^n, q^n, μ^n) converging to the saddle-point.

ALG2:

- $(\phi^{n-1}, q^{n-1}, \mu^n)$ are given.
- Step A: Find ϕ^n such that :

$$L_r(\phi^n, q^{n-1}, \mu^n) \leq L_r(\phi, q^{n-1}, \mu^n), \quad \forall \phi. \quad (47)$$

- Step B: Find q^n such that :

$$L_r(\phi^n, q^n, \mu^n) \leq L_r(\phi, q, \mu^n), \quad \forall q. \quad (48)$$

- Step C : Do

$$\mu^{n+1} = \mu^n + r(\nabla_{t,x}\phi^n - q^n) \quad (49)$$

(where $r > 0$ is the parameter of the Augmented Lagrangian).

- Go back to step A.

Step A and B are simply a relaxation method for the minimization part of the saddle-point problem. Step C is a gradient step for the dual problem.

Step A

To get Step A, we differentiate L_r with respect to ϕ and get for ϕ^n :

$$G(\phi) + r \langle \nabla_{t,x}\phi^n - q^{n-1}, \nabla_{t,x}\phi \rangle + \langle \mu^n, \nabla_{t,x}\phi \rangle = 0, \quad \forall \phi.$$

After integrating by part in space and time, we see that this is the variational formulation of the space-time Laplace equation

$$-r\Delta_{t,x}\phi^n = \nabla_{t,x} \cdot (\mu^n - rq^{n-1}) \quad (50)$$

with periodic boundary conditions in space and Neumann boundary conditions in time :

$$r\partial_t\phi^n(0, \cdot) = \rho_0 - \rho^n(0, \cdot) + ra^{n-1}(0, \cdot), \quad (51)$$

$$r\partial_t\phi^n(T, \cdot) = \rho_T - \rho^n(T, \cdot) + ra^{n-1}(T, \cdot). \quad (52)$$

Recall that $\mu^n = \{\rho^n, m^n\}$ and $q^{n-1} = \{a^{n-1}, b^{n-1}\}$.

Note that this Neumann problem is well posed since

$$\int_D [\rho_0 - \rho_T] = 0.$$

In practice, for programming simplicity, we use the perturbed Laplace equation

$$-r\Delta_{t,x}\phi^n + r\epsilon_2\phi^n = \nabla_{t,x} \cdot (\mu^n - rq^{n-1})$$

where ϵ_2 is a small positive parameter.

Step B

We cannot differentiate L_r with respect to q and q^n is simply obtained by solving

$$\inf_q [F(q) + \frac{r}{2} \langle \nabla_{t,x}\phi^n - q, \nabla_{t,x}\phi^n - q \rangle + \langle \mu^n, \nabla_{t,x}\phi^n - q \rangle],$$

which is equivalent to :

$$\inf_{q \in K} \langle \nabla_{t,x}\phi^n + \frac{\mu^n}{r} - q, \nabla_{t,x}\phi^n + \frac{\mu^n}{r} - q \rangle.$$

It is important to notice that this minimization can be performed pointwise in space and time. Indeed, let us set :

$$p^n(t, x) = \{\alpha^n(t, x), \beta^n(t, x)\} = \nabla_{t,x}\phi^n(t, x) + \frac{\mu^n(t, x)}{r}.$$

Then $q^n(t, x) = \{a^n(t, x), b^n(t, x)\}$ is obtained by solving in (a, b) :

$$\inf \left\{ (a - \alpha^n(t, x))^2 + |b - \beta^n(t, x)|^2, \quad a + \frac{|b|^2}{2} \leq 0 \right\}$$

This turns out to be simple one dimensional projection problem which can be computed analytically or using Newton's method.

Step C

Step C is simply the pointwise update :

$$\mu^{n+1}(t, x) = \mu^n(t, x) + r(\nabla_{t,x}\phi^n(t, x) - q^n(t, x)).$$

Cost and convergence criterium.

Among these three steps, only Step A is global. This means that the cost of Step B and C are of order $O(N)$ where N is the number of points of the space time lattice. The Laplace equation (step A) can be solved in $O(N \text{Log} N)$ operations. The cost of this methods is therefore of order $N \text{Log} N$ times the number

of iterations in n needed for converge.

We do not have theoretical estimates on the speed of convergence of the method. To be able to produce numerical estimates and also for the practical purpose of stopping the computation we need to define a convergence criterium. The optimality conditions (37) are useful for that purpose. We can indeed use the residual of the Hamilton-Jacobi equation (11), namely

$$res^n = \partial_t \phi^n + \frac{|\nabla_x \phi^n|^2}{2}$$

which is a by-product of the algorithm. This quantity converges to 0 as we approach the solution of problem. The normalized convergence criterium used is

$$crit^n = \sqrt{\frac{\int_0^T \int_D \rho^n |res^n|}{\int_0^T \int_D \rho^n |\nabla_x \phi^n|^2}}. \quad (53)$$

5 Numerical results.

We present numerical tests performed on the unit square with periodic boundary conditions in space. The space-time domain is discretized using a regular $32 \times 32 \times 31$ lattice. The parameters of the method are taken as $\epsilon_2 = 0.001$ and $r = 1$. As usual for gradient method convergence rate quickly decays. However, a moderate number of iterations (about 30 for smooth data and few hundreds for piecewise constant data) is enough to get good approximate solutions in practice. We show for different time steps the level curves of the approximate solution ρ . The final value of ρ at time step 31 always match ρ_T .

Test 1

The exact solution of this problem set in free space is the translation of a gaussian density (figure 1). There is no noticable effect of the periodic boundary conditions.

Test 2

Because of the periodic boundary conditions, this experiment amounts to shift along the diagonal an infinite lattice of gaussian functions. The optimal transfer is not a simple translation as could be primarily thought but rather prefers to split each gaussian functions into four pieces, sending each of them to the nearest corner (figure 2).

Test 3

Here, we perform a test similar to Test 1, but with a step function fitting an ellipse and a larger translation. As we use periodic boundary conditions in space, a part of the mass is transferred across the periodic boundaries (figure 3). To get a higher resolution, a $32 \times 64 \times 64$ grid has been used, with 400 iterations.

Test 4

Here we perform both translation and rotation of a step function fitting an ellipse. Once again, there is a substantial transfer of mass across the boundary due to the periodic conditions (figure 4). Small errors produce scattered pebbles.

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