Activity Report 2013

Exploratory Action MOKAPLAN

Numerical methods for the Monge-Kantorovitch problem, applications and extensions
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Keywords: Optimal Mass Transportation, Monge-Ampère, Wassstein Distance, Economic Models

Creation of the Exploratory Action: 2013 January 01.

1. Members

Research Scientist
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External Collaborators
Guillaume Carlier [Co-Team leader, Univ. Paris IX, Professor, from Jan 2013, HdR]
Adam Oberman [Univ. Mc Gill (Canada), Professor, HdR]
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Engineers
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Nicolas Bonne [from Jun 2013 until Aug 2013]

2. Overall Objectives

2.1. Introduction

Over the last twenty years, Optimal Mass Transportation has played a major role in PDEs, geometry, functional inequalities as well as in modelling and applied fields such as image fluid mechanics, image processing and economics. This trend shows no sign of slowing and the field is still extremely active. However, the numerics remain underdeveloped, but recent progress in this new field of numerical Optimal Mass Transportation raise hope for significant advances in numerical simulations.

Mokaplan objectives are to design, develop and implement these new algorithms with and emphasis on economic applications.
2.2. Highlights of the Year

The paper [6] resolves numerically the Monge-Ampère formulation of the Optimal Transportation problem with quadratic cost with the correct “second boundary value” boundary conditions. It is worth pointing that this has been an open problem for a while. The same paper proposes a fast and robust Newton method (empirically linear) which can be applied to degenerate cases. This potentially means progress in many applications of Optimal Mass Transportation. The method has, for instance, been reimplemented in [72] by TU Eindhoven researchers in collaboration with Philips Lighting Labs to simulate the design of reflectors. In 2013, the method was the topic of invited presentations at the Collège de France applied math seminar, at MSRI (UC Berkeley) special program on Optimal Mass Transportation and at SIAM annual conference on PDE analysis.

3. Research Program

3.1. Context

Optimal Mass Transportation is a mathematical research topic which started two centuries ago with Monge’s work on “des remblais et déblais”. This engineering problem consists in minimizing the transport cost between two given mass densities. In the 40’s, Kantorovitch [54] solved the dual problem and interpreted it as an economic equilibrium. The Monge-Kantorovitch problem became a specialized research topic in optimization and Kantorovitch obtained the 1975 Nobel prize in economics for his contributions to resource allocations problems. Following the seminal discoveries of Brenier in the 90’s [23], Optimal Transportation has received renewed attention from mathematical analysts and the Fields Medal awarded in 2010 to C. Villani, who gave important contributions to Optimal Transportation and wrote the modern reference monograph [75], arrived at a culminating moment for this theory. Optimal Mass Transportation is today a mature area of mathematical analysis with a constantly growing range of applications (see below).

In the modern Optimal Mass Transportation problem, two probability measures or "mass" densities : $\rho_i(x_i) := \rho_i(x_i) \, dx_i, \; i = 0, 1$ such that $\rho_i \geq 0, \, \int_{X_i} \rho_0(x_0) \, dx_0 = \int_{X_1} \rho_1(x_1) \, dx_1 = 1, \; X_i \subset \mathbb{R}^n$. They are often referred to, respectively, source and target densities, support or spaces. The problem is the minimization of a transportation cost, $\mathcal{J}(M) = \int_{X_0} c(x, M(x)) \, \rho_0(x) \, dx$ where $c$ is a displacement ground cost, over all volume preserving maps $M \in \mathcal{M} = \{ M : X_0 \to X_1, \; M \# d\rho_0 = d\rho_1 \}$. Assuming that $M$ is a diffeomorphism, this is equivalent to the Jacobian equation $\det(DM(x)) \rho_1(M(x)) = \rho_0(x)$. Most of the modern Optimal Mass Transportation theory has been developed for the Euclidean distance squared cost $c(x, y) = \| x - y \|^2$ while the historic monge cost was the simple distance $c(x, y) = \| x - y \|$.

In the Euclidean distance squared ground cost, the problem is well posed and in the seminal work of Brenier [24], the optimal map is characterized as the gradient of a convex potential $\phi^*$ : $\mathcal{J}(\nabla \phi^*(x)) = \min_M \mathcal{J}(M)$. A formal substitution in the Jacobian equation gives the Monge-Ampère equation $\det(D^2 \phi^*) \rho_1(\nabla \phi^*(x)) = \rho_0(x)$ complemented by the second boundary value condition $\nabla \phi^*(X_0) \subset X_1$. Caffarelli [29] used this result to extend the regularity theory for the Monge-Ampère equation. He noticed in particular that Optimal Mass Transportation solutions, now called Brenier solutions, may have discontinuous gradients when the target density support $X_1$ is non convex and are therefore weaker than the Monge-Ampère potentials associated to Alexander measure [50] for a review of the different notions of Monge-Ampère solutions. The value function $\sqrt{\mathcal{J}(\nabla \phi^*)}$ is also known to be the Wasserstein distance $W_2(\rho_0, \rho_1)$ on the space of probability densities, see [75]. The Computational Fluid Dynamic formulation proposed by Brenier and Benamou in [2] introduces a time extension of the domain and leads to a convex but non smooth optimization problem : $\mathcal{J}(\nabla \phi^*) = \min_{(\rho, V) \in C} \int_0^1 \int_X \frac{1}{2} \rho(t, x) \| V(t, x) \|^2 \, dx \, dt$ with constraints : $C = \{ (\rho, V), \; s.t. \; \partial_t \rho + \text{div}(\rho V) = 0, \; \rho(0, 1, \cdot) = \rho(0, 1, \cdot) \}$. The time curves $t \to \rho(t, \cdot)$ are geodesics between $\rho_0$ and $\rho_1$ for the Wasserstein distance. This formulation is a limit case of Mean Fields games [55], a large class of economic models introduced by Lasry and Lions. The Wasserstein distance and its connection to Optimal Mass Transportation also appears in the construction of semi-discrete Gradient Flows. This notion known as KJO gradient flows after its authors in [52] is a popular tool to study
Figure 1. Top: the color map of the mass to be transported to a constant mass density ellipse, dark blue is no mass - Bottom: the deformation under the optimal transportation map of the initial computational cartesian grid on the top square.
4. Application Domains

4.1. Continuous models in Economy

- As already mentioned the CFD formulation is a limit case of simple variational Mean-Field Games (MFG) [55]. MFG is a new branch of game theory recently developed by J-M. Lasry and P-L. Lions. MFG models aim at describing the limiting behavior of stochastic differential equations when the number of players tends to infinity. They are specifically designed to model economic problems where a large number of similar interacting agents try to maximize/minimize a utility/cost function...
which takes into account global but partial information on the game. The players in these models are individually insignificant but they collectively have a significant impact on the cost of the other players. Dynamic MFG models often lead to a system of PDEs which consists of a backward Hamilton-Jacobi Bellman equation for a value function coupled with a forward Fokker-Planck equation describing the space-time evolution of the density of agents.

- In microeconomics, the principal-agent problem [74] with adverse selection plays a distinguished role in the literature on asymmetric information and contract theory (with important contributions from several Nobel prizes such as Mirrlees, Myerson or Spence) and it has many important applications in optimal taxation, insurance, nonlinear pricing. The problem can be reduced to the maximization of an integral functional subject to a convexity constraint This is an unusual calculus of variations problem and the optimal price can only be computed numerically. Recently, following a reformulation of Carlier [11], convexity/well-posedness results of McCann, Figalli and Kim [42], connected to optimal transport theory, showed that there is some hope to numerically solve the problem for general utility functions.

- In [8] a class of games are considered with a continuum of players for which Cournot-Nash equilibria can be obtained by the minimisation of some cost, related to optimal transport. This cost is not convex in the usual sense in general but it turns out to have hidden strict convexity properties in many relevant cases. This enables us to obtain new uniqueness results and a characterisation of equilibria in terms of some partial differential equations, a simple numerical scheme in dimension one as well as an analysis of the inefficiency of equilibria. The mathematical problem has the structure of one step of the JKO gradient flow method.

- Many relevant markets are markets of indivisible goods characterized by a certain quality: houses, jobs, marriages... On the theoretical side, recent papers by Ekeland, McCann, Chiappori [34] showed that finding equilibria in such markets is equivalent to solving a certain optimal transport problem (where the cost function depends on the sellers and buyers preferences). On the empirical side, this allows for trying to recover information on the preferences from observed matching; this is an inverse problem as in a recent work of Galichon and Salanié [47] [48] Interestingly, these problems naturally lead to numerically challenging variants of the Monge-Kantorovich problem: the multi-marginal OT problem and the entropic approximation of the Monge-Kantorovich problem (which is actually due to Schrödinger in the early 30’s).

### 4.2. Finance

The Skorohod embedding problem (SEP) consists in finding a martingale interpolation between two probability measures. When a particular stochastic ordering between the two measures is given, Galichon et al [46] have shown that a very natural variational formulation could be given to a class of problems that includes the SEP. This formulation is related to the CFD formulation of the OT problem [2] and has applications to *model-free bounds of derivative prices in Finance*. It can also be interpreted as a a multi marginal Optimal Mass Transportation with infinitely many marginals [69].

### 4.3. Congested Crowd motion

The volume preserving property appears naturally in this context where motion is constrained by the density of player.

- Optimal Mass Transportation and MFG theories can be an extremely powerful tool to attack some of these problems arising from spatial economics or to design new ones. For instance, various urban/traffic planning models have been proposed by Buttazzo, Santambrogio, Carlier,[9] [28] [20]) in recent years.

- Many models from PDEs and fluid mechanics have been used to give a description of *people or vehicles moving in a congested environment*. These models have to be classified according to the dimension (1D model are mostly used for cars on traffic networks, while 2D models are most suitable
for pedestrians), to the congestion effects ("soft" congestion standing for the phenomenon where high densities slow down the movement, "hard" congestion for the sudden effects when contacts occur, or a certain threshold is attained), and to the possible rationality of the agents Maury et al [59] recently developed a theory for 2D hard congestion models without rationality, first in a discrete and then in a continuous framework. This model produces a PDE that is difficult to attack with usual PDE methods, but has been successfully studied via Optimal Mass Transportation techniques again related to the JKO gradient flow paradigm.

4.4. Astrophysics

In [44] and [25], the authors show that the deterministic past history of the Universe can be uniquely reconstructed from the knowledge of the present mass density field, the latter being inferred from the 3D distribution of luminous matter, assumed to be tracing the distribution of dark matter up to a known bias. Reconstruction ceases to be unique below those scales – a few Mpc – where multi-streaming becomes significant. Above 6 Mpc/h we propose and implement an effective Monge-Ampere-Kantorovich method of unique reconstruction. At such scales the Zel’dovich approximation is well satisfied and reconstruction becomes an instance of optimal mass transportation. After discretization into N point masses one obtains an assignment problem that can be handled by effective algorithms with not more than cubic time complexity in N and reasonable CPU time requirements. Testing against N-body cosmological simulations gives over 60% of exactly reconstructed points.

4.5. Image Processing and inverse problems

The Wasserstein distance between densities is the value function of the Optimal Mass Transportation problem. This distance may be considered to have "orthogonal" properties to the widely used least square distance. It is for instance quadratic with respect to dilations and translation. On the other hand it is not very sensitive to rigid transformations, [64] is an attempt at generalizing the CFD formulation in this context. The Wasserstein distance is an interesting tool for applications where distances between signals and in particular oscillatory signals need to be computed, this is assuming one understand how to transform the information into positive densities.

- Tannenbaum and co-authors have designed several variants of the CFD numerical method and applied it to warping, morphing and registration (using the Optimal Mass Transportation map) problems in medical imaging. [76] [17]
- Gabriel Peyre and co-authors [73] have proposed an easier to compute relaxation of the Wasserstein distance (the sliced Wasserstein distance) and applied it to two image processing problems: color transfer and texture mixing.
- Froese Engquist [40] use a Monge-Ampère Solver to compute the Wasserstein distance between synthetic 2D Seismic signals (After some transformations). Applications to waveform inversion and registration are discussed and simple numerical examples are presented.

4.6. Meteorology and Fluid models

In, [22] Brenier reviews in a unified framework the connection between optimal transport theory and classical convection theory for geophysical flows. Inspired by the numerical model proposed in [17], the starting point is a generalization of the Darcy-Boussinesq equations, which is a degenerate version of the Navier-Stokes-Boussinesq (NSB) equations. In a unified framework, he relates different variants of the NSB equations (in particular what he calls the generalized hydrostatic-Boussinesq equations) to various models involving optimal transport and the related Monge-Ampère equation. This includes the 2D semi-geostrophic equations [51] [38] [37] [4] [57] and some fully nonlinear versions of the so-called high-field limit of the Vlasov-Poisson system [65] and of the Keller-Segel system for chemotaxis [53] [33].
4.7. Mesh motion/Lagrangian methods

The necessity to preserve areas/volumes is an intrinsic feature of mesh deformations more generally Lagrangian numerical methods. Numerical method of Optimal Mass Transportation which preserve some notions of convexity and as a consequence the monotonicity of the computed transport maps can play a role in this context, see for instance [32] [35] [56].

4.8. Density Functional Theory (DFT)

The precise modeling of electron correlations continues to constitute the major obstacle in developing high-accuracy, low-cost methods for electronic structure computations in molecules and solids. The article [36] sheds new light on the longstanding problem of how to accurately incorporate electron correlation into DFT, by deriving and analyzing the semiclassical limit of the exact Hohenberg-Kohn functional with the single-particle density $\rho$ held fixed. In this limit, in the case of two electrons, the exact functional reduces to a very interesting functional that depends on an optimal transport map $M$ associated with a given density $\rho$. The limit problem is known in the DFT literature with the optimal transport map being called a correlation function or a co-motion function, but it has not been rigorously derived, and it appears that it has not previously been interpreted as an optimal transport problem. The article [36] thereby links for the first time DFT, which is a large and very active research area in physics and chemistry, to optimal transportation theory, which has recently become a very active area in mathematics. Numerics are still widely open [26].

5. Software and Platforms

5.1. CFD based MK solvers

5.1.1. Platforms

The core of the ALG2 algorithm [43] for the CFD formulation of the Optimal Mass Transportation problem and many of its generalization is a Poisson solver. Then each problem calls for different but simple modifications the point wise minimization of a given Lagrangian function. We have written such a FreeFem ALG2 platform and are plan to implement a parallel version on Rocquencourt Inria cluster.

5.2. MA based Optimal Mass Transportation solvers

5.2.1. Platforms

Monotone discretisations of the Monge-Ampère operator (the determinant of a Hessian function) is the core of Monge-Ampère Optimal Mass Transportation solvers but is also a useful tool for convexity constraints in infinite dimensional optimization and JKO gradient flows. We are implementing in F90 and comparing several monotone schemes. These modules could be reused in different applications.

6. New Results

6.1. Monge-Ampère solver for the Mass Transportation problem and extensions

- Benamou, Froese (Univ. of Texas at Austin) - We design a scheme for Aleksandrov solution of Optimal Mass Transportation between atomic measure and continuous densities. The idea is to couple the notion of viscosity solution with an adapted sub gradient discretization at dirac points where the notion of Aleksandrov solution is relevant. This would offer a ”PDE” alternative to the classical gradient methods based on costly computational geometry tools [61].
• Benamou, Collino, Mirebeau (Univ. Paris IX, CNRS) - A new variational formulation of the determinant of a semi-definite positive matrix has been proposed based on the ideas developed in [60]. This leads to a monotone discretisation of the Monge-Ampère operator. A Newton method preserving convexity is currently being tested. The new scheme is more accurate than the wide stencil, currently the state of the art of monotone scheme for the Monge-Ampère equation.

• Benamou, Froese (Univ. of Texas at Austin), Oberman (Univ. Mc Gill) - When the Optimal Mass Transportation data is not balanced, i.e. the densities do not have equal mass. A natural extension of the optimal transport has been proposed by McCann and Caffarelli [30] and revisited by Figalli [41]. It is formulated as an obstacle problem which automatically select the portion of mass corresponding to Optimal Mass Transportation. The numerical resolution of this problem is open and we believe ideas linked the state constraint reformulation contained in paper [6] may be applied to obtain a tractable reformulation.

6.2. Variational problems under divergence constraint - Alg2

• Benamou, Bonne, Carlier - Dynamic problems: we have extended the Augmented Lagrangian method used for the CFD formulation of the Optimal Mass Transportation to Mean Field Games that is for the optimal control of the continuity equation. A freefem Code has been implemented.

• Benamou, Carlier - Static problems with a divergence constraint. We have also extended the Augmented Lagrangian method to static problem where a space divergence constraint appears. This includes the delicate case of the original Monge Optimal Mass Transportation cost (cost=distance) and also Wardrop equilibria in congested transport and related degenerate elliptic equations, like the $p$-Laplacian operator. A freefem Code has been implemented.

6.3. Multi-marginal problems

• [Carlier, Oberman (Univ. Mc Gill), Oudet (Univ. of Grenoble) - New numerical methods for the Wasserstein barycenter and related multi-marginals problems were investigated [49]. A first method uses linear programming, in an implementation that was more efficient than expected. A second method takes advantage of the quadratic structure and leads to an efficient algorithm that can be used in texture synthesis problems arising in image processing.

• Benamou, Carlier, Nenna Extension of the CFD formulation and the ALG2 algorithm to the multi marginal problem with quadratic cost (Barycenter).

6.4. JKO gradient flow numerics

• Benamou, Carlier, Merigot (Univ. of Grenoble, CNRS), Oudet (Univ. of Grenoble) A large class of non-linear continuity equations with confinement and/or possibly non local interaction potential can be considered as semi discrete gradient flows with respect to the Euclidean Wasserstein distance. The numerical resolution of such problem in dimension 2 and higher is open. Our approach is based on two remarks : the reformulation of the optimization problem in terms of Brenier potential seems to behave better. This introduces a Monge-Ampère operator in the cost functional which needs a monotone discretization in order to preserve the convexity at the discrete level. The first numerical results are very encouraging.

• Benamou, Carlier, Agueh (Univ. of Victoria) Splitting methods for kinetic equations, we try to use one JKO step to deal with the non-linear velocity advection part of kinetic equations [31]. This seems to be relevant to granular media equation [16], and also may offer a completely new method for Liouville equations arising from Geometrical Optics [19].
Figure 2. Monge transport flow between sinks and sources.
Figure 3. Congested transport flows between sink and source.
Figure 4. Texture mixing with Wasserstein barycenters, from top to bottom three densities and their barycenter.
Figure 5. One step of Wasserstein JKO gradient flow for the classical entropy (our numerical method) compared to traditional Finite Difference of the heat equation. Left the initial heat profile, right the heat profile after one time step for both methods.
7. Partnerships and Cooperations

7.1. National Initiatives

7.1.1. ANR

Jean-David Benamou is the coordinator of the ANR ISOTACE (Interacting Systems and Optimal Transportation, Applications to Computational Economics) ANR-12-MONU-0013 (2012-2016). The consortium explores new numerical methods in Optimal Transportation and Mean Field Game theory with applications in Economics and congested crowd motion. Four extended seminars have been organized/co-organized by Mokaplan. Check [https://project.inria.fr/isotace/news](https://project.inria.fr/isotace/news). Christophe Duquesne (Aurigetech) is a software and mobility consultant hired on the ANR budget. He helps the consortium to develop its industrial partnerships.

7.2. International Initiatives

7.2.1. Informal International Partners

Mokaplan has strong links with several Canadian researchers (Oberman, Froese, Agueh, Pass). In July 2013, Oudet, Carlier, Agueh, Pass, Oberman, Froese and Benamou gathered in Banff for a "focused research group" week: [http://www.birs.ca/events/2013/focussed-research-groups/13frg167](http://www.birs.ca/events/2013/focussed-research-groups/13frg167). The meeting was productive and several new collaborations were started on the occasion which are listed in the objectives of this proposal.

7.3. International Research Visitors

7.3.1. Visits of International Scientists

- Brendan Pass (U. of Alberta).
- Brittany Froese (U. Texas at Austin).
- Giuseppe Buttazzo (U. Pisa).

7.3.1.1. Internships

- Nicolas Bonne extended the ALG2 used in the CFD approach to Optimal Mass Transportation to build a numerical method for Mean Field Games models.

8. Dissemination

8.1. Teaching - Supervision - Juries

8.1.1. Teaching

- Licence : Guillaume Carlier, Analyse complexe, 30hETD, Dauphine, L3,
- Master 2: Guillaume Carlier, Mean-Field-Games, 18hETD, Dauphine, M2,
- Doctorat : Guillaume Carlier, cours Optimization with divergence constraints and applications, Pisa, Italie, 12h.

8.1.2. Supervision

PhD in progress : Luca Nenna, 01/10/2013, J.D. Benamou & G. Carlier
PhD in progress : Maxime Laborde (01/09/2013) and Romeo Hatchi (01/09/2012), G. Carlier

8.1.3. Juries
Jean-David Benamou reviewer of PhD : Nicolas Bonnote, Unidimensional and Evolution Method for Optimal Transportation, Université Paris Sud, dec. 16 2013. Advisors : L. Ambrosio and F. Santambrogio

Guillaume Carlier jury member for the PhD of Vincent Nolot (Dijon), Miryana Grogorova (Paris 7) and Beatrice Acciaio (Vienna, reviewer), HDR committees: Pierre Bousquet (Marseille) and Naila Hayek (Paris 1).

8.2. Popularization

Jean-David Benamou run a Ipython Notebook web site https://mathmarx.rocq.inria.fr:9999 on which simple Optimal Mass Transportation algorithm are coded in python and can be tested and modified.

9. Bibliography

Major publications by the team in recent years


Publications of the year

Articles in International Peer-Reviewed Journals


Research Reports


References in notes


