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Numerical Analysis

Optimal transport, shape optimization and global minimization

Bijan Mohammadi

Institut de mathématiques et de modélisation de Montpellier, Université Montpellier II, CC51, 34095 Montpellier, France

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Abstract

We present the numerical solution of general optimal transport problems through global minimization formulated as solution of boundary value problems. The paper is not on optimal transport but aims to show that the optimization problem behind needs global solutions. One gives also interest to the variable sign right-hand-side case with application to shape optimization for surfaces at given curvature. Both the positive and variable sign problems have local minima, but have unique global solution. ***To cite this article: B. Mohammadi, C. R. Acad. Sci. Paris, Ser. I 344 (2007).***

Résumé

Transport optimal généralisé, optimisation de formes et minimisation globale. Nous présentons la résolution de problème de transport optimal généralisé comme solution d'une minimisation globale basée sur la solution de problèmes à valeurs aux limites. On s'intéresse au cas de second membre à signe variable dans l'équation de Monge–Ampère, avec comme application l'optimisation de formes de surfaces à courbure donnée. Les problèmes ont toujours des minima locaux mais l'optimum global est unique. ***Pour citer cet article : B. Mohammadi, C. R. Acad. Sci. Paris, Ser. I 344 (2007).***

Version française abrégée

La solution numérique de l'équation de Monge–Ampère dans le cas général n'est pas possible avec les méthodes numériques classiques pour les EDP. En effet, ces méthodes sont conçues différemment pour chaque type d'EDP. Dans le cas général, notre équation nonlinéaire change de type suivant le signe du second membre. Nous montrons qu'une minimisation globale est nécessaire pour la solution du problème de minimisation associé. Les méthodes numériques actuellement utilisées sont basées sur des itérations de point fixe de type Newton [9] ou des méthodes de minimisation pour une formulation Lagrangien augmenté [9,4,2]. Elles ne peuvent donc pas résoudre ce problème car capturées par des minima locaux.

E-mail addresses: bijan.mohammadi@univ-montp2.fr, bijan.mohammadi@universite-montpellier2.eu.

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1. Introduction

The mass transport problem was first considered by Monge in 1780 in his "*mémoire sur les remblais et les déblais*" and revisited by Kantorovich in 1948 [8]. This problem has regained interest more recently as it models wide ranges of applications from image processing and physics to economics (see [10,2,3] for exhaustive lists of references).

A numerical solution of the Monge–Ampère equation (MAE) with classical methods for PDE fails as this equation changes type following the sign of its right-hand-side (the PDE is elliptic if it is strictly positive, parabolic if it vanishes and hyperbolic if strictly negative).

Current numerics only target strictly positive right-hand-side and use either fixed point Newton type iterations [9] or minimization approaches for an augmented Lagrange formulation [4,2]. We would like to propose a new way to solve the MAE in the general case and show its application to shape design to find surfaces with given curvature. The optimal transport problem corresponds to the particular case of strictly positive curvature.

We would like here to show the importance of a global minimization approach to solve the MAE. Indeed, one shows that the associated minimization problem, even for the positive sign case, has local minima.[1] One can therefore expect difficulties in solving this problem with classical fixed point iterations (Newton, ...).

2. Optimal transport

Consider two bounded, positive and integrable functions ρ_0 and ρ_1 with compact support in $\mathbb{R}^n$ such that

$$\int_{\mathbb{R}^n} \rho_0 = \int_{\mathbb{R}^n} \rho_1. \tag{1}$$

One would like to find the application $M : \mathbb{R}^n \to \mathbb{R}^n$ realizing the transformation from ρ_0 to ρ_1 minimizing, for instance,

$$\int_{\mathbb{R}^n} \big\|x - M(x)\big\|^2 \rho_0(x) \tag{2}$$

and such that for all continuous function φ

$$\int_{\mathbb{R}^n} \rho_0(x)\varphi\big(M(x)\big) = \int_{\mathbb{R}^n} \rho_1(x)\varphi(x). \tag{3}$$

One knows that there is a unique $M = \nabla\psi$ with ψ a convex potential satisfying (2) [10]. In addition, if the densities are strictly positive and continuous then one can look for ψ solution of MAE ($H(\psi)$ being the Hessian of ψ and $\det(H)$ its determinant),

$$\det\big(H\big(\psi(x)\big)\big) = \frac{\rho_0(x)}{\rho_1(\nabla\psi(x))}. \tag{4}$$

Solution to this problem can also come from a continuous time method minimizing some distance function between densities ρ_0 and ρ_1. The Wasserstein distance provides solution for (4). It can be defined via a conservative flow:

$$d_W(\rho_0, \rho_1)^2 = \inf \int_{\mathbb{R}^n} \int_0^1 \rho(t,x)\big\|v(t,x)\big\|^2 \tag{5}$$

where (ρ, v) verifies the following conservation law:

$$\rho_t + \nabla\cdot(\rho v) = 0, \quad \rho(0,x) = \rho_0(x), \quad \rho(1,x) = \rho_1(x). \tag{6}$$

This is therefore a minimization problem with equality constraint. Optimality condition gives [2]

$$M = \nabla\psi = \nabla\phi + x \tag{7}$$

[1] This is not incompatible with the uniqueness of the solution.

where

$$\phi_t + 1/2|\nabla\phi|^2 = 0, \tag{8}$$

$$\rho_t + \nabla(\rho\nabla\phi) = 0, \quad \rho(0,x) = \rho_0(x), \quad \rho(1,x) = \rho_1(x) \tag{9}$$

with ϕ the Lagrange multiplier for the conservation constraint (6). This can be solved with an augmented Lagrange formulation minimizing the Eikonal equation residual under constraint (9) [2,5,4].

Here, we would like to go one step further and solve the case of variable sign determinant in (4). Unlike in the positive sign case, the minimization problem for the residual of (4) cannot be solved using formulation (5)–(9). In addition, we will see that this minimization problem has local minima and a global optimization approach is required.

In the following we consider the MAE for the definition of a 3D surface from a given curvature minimizing $J(\psi) = \|\psi_{xx}\psi_{yy} - \psi_{xy}^2 - f(x,y)\|$ where ψ is a given shape parameterization.

3. Global optimization

Consider the minimization of a functional $J(\psi) \geqslant 0, \ \psi \in \mathcal{O}_{ad}$. We suppose the problem admissible (i.e. there exist at least one solution ψ_m to the problem: $J(\psi_m) = J_m$). Most minimization algorithms can be seen as discretizations of [6]:

$$M\big(\psi(\zeta)\big)\psi_\zeta = -d\big(\psi(\zeta)\big), \quad \psi(\zeta = 0) = \psi_0. \tag{10}$$

M is aimed to be positive definite and $M^{-1}d$ is built to be an admissible direction. Global solution of (10) means, for instance, finding $\psi(1)$ such that

$$M\big(\psi(\zeta)\big)\psi_\zeta = -d\big(\psi(\zeta)\big), \quad \psi(0) = \psi_0, \quad J(\psi(1)) = 0. \tag{11}$$

This is an over-determined boundary value problem and it tells us why one should not solve global optimization problems with methods which are discrete form of Cauchy problems for first order differential systems.[2] Except if one can provide an initial condition in the attraction basin of the global optimum. Hence, in the context of global optimization the initial condition ($\psi(0) = \psi_0$), is misleading. On the other hand, one would like to realize the optimality condition ($J'(\psi(1)) = 0$). Finally, to remove overdetermination we consider the following second order system [1] with two final conditions:

$$\eta\psi_{\zeta\zeta} + M\big(\psi(\zeta)\big)\psi_\zeta = -d\big(\psi(\zeta)\big), \qquad J\big(\psi(1)\big) = J'\big(\psi(1)\big) = 0. \tag{12}$$

This can be solved using solution techniques for BVPs with free surface [7]. An analogy can be given with the problem of finding the interface between water and ice which is only implicitly known through the iso-value of zero temperature.

3.1. Recursive minimization algorithm

Global optimization of J has a solution if, for a given precision ε in the functional, one can build at least one trajectory $(\psi(t), 0 \leqslant t \leqslant T_\varepsilon)$ passing in finite time T_ε enough close to ψ_m. In what follows, these trajectories will be generated by first or second order Cauchy problems starting from an initial value v. These will be denoted $(\psi_v(t), 0 \leqslant t \leqslant T_\varepsilon, v \in \mathcal{O}_{ad})$. Existing minimization methods build such trajectories in discrete form. This can be summarized as:

$$\forall\varepsilon > 0, \ \exists(v, T_\varepsilon) \in \mathcal{O}_{ad} \times [0, +\infty[\quad \text{such that} \quad J\big(\psi_v(T_\varepsilon)\big) - J_m \leqslant \varepsilon. \tag{13}$$

If J_m is unknown T_ε defines the maximum calculation complexity wanted. In these cases, setting $J_m = -\infty$, one retains the best solution obtained over $[0, T_\varepsilon]$. In other words, one solves:

$$\forall(\varepsilon, T_\varepsilon) \in \mathbb{R}^+ \times [0, +\infty[, \quad \exists(v,\tau) \in \mathcal{O}_{ad} \times [0, T_\varepsilon] \quad \text{such that} \quad J\big(\psi_v(\tau)\big) - J_m \leqslant \varepsilon. \tag{14}$$

Below, we propose, a recursive algorithm to solve (13) or (14):

[2] Eq. (6) already shows a formulation involving a boundary value problem.

Given $\varepsilon > 0$, J_m and $0 \leqslant T_\varepsilon < \infty$, we minimize the functional $h_{\varepsilon,T_\varepsilon,J_m} : \mathcal{O}_{ad} \to \mathbb{R}^+$ below:

$$h_{\varepsilon,T,J_m}(v) = \min_{\psi_v(\tau)\in\mathcal{O}_{ad},\, \tau\in[0,T]} \big(J\big(\psi_v(\tau)\big) - J_m\big). \tag{15}$$

Hence, global minimization becomes a nested minimization problem where one looks for v to provide a better initial value to generate the trajectory $(\psi_v(\tau), 0 \leqslant \tau \leqslant T_\varepsilon)$ (i.e. passing closer to ψ_m). Below, one shows a recursive solution algorithm to this problem (denote $h_{\varepsilon,T_\varepsilon,J_m}$ by h).

Consider the following algorithm $A_1(v_1, v_2)$:

- $(v_1, v_2) \in \mathcal{O}_{ad} \times \mathcal{O}_{ad}$ given
- Find $v \in \operatorname{argmin}_{w\in\mathcal{O}(v_1,v_2)} h(w)$ where $\mathcal{O}(v_1, v_2) = \{v_1 + t(v_2 - v_1), t \in \mathbb{R}\} \cap \mathcal{O}_{ad}$ using a line search method
- return v

The linesearch minimization in A_1 is defined by the user. It may fail. For instance, a secant method degenerates on plateaux and critical points. In this case, in order to have a multidimensional search, we add an external layer to the algorithm A_1 minimizing $h'(v') = h(A_1(v', w'))$ with w' chosen randomly in $\mathcal{O}_{ad}$. This is the only stochastic feature of the algorithm.

This leads to the following two-layer algorithm $A_2(v'_1, v'_2)$:

- $(v'_1, v'_2) \in \mathcal{O}_{ad} \times \mathcal{O}_{ad}$ given
- Find $v' \in \operatorname{argmin}_{w\in\mathcal{O}(v'_1,v'_2)} h'(w)$ where $\mathcal{O}(v'_1, v'_2) = \{v'_1 + t(v'_2 - v'_1), t \in \mathbb{R}\} \cap \mathcal{O}_{ad}$ using a line search method
- return v'

Again, the line search minimization in A_2 is user-defined. This construction can be pursued by building recursively $h^i(v_1^i) = h^{i-1}(A_{i-1}(v_1^i, v_2^i))$, with $h^1(v) = h(v)$ and $h^2(v) = h'(v)$ where $i = 1, 2, 3, \ldots$ denotes external layers. Due

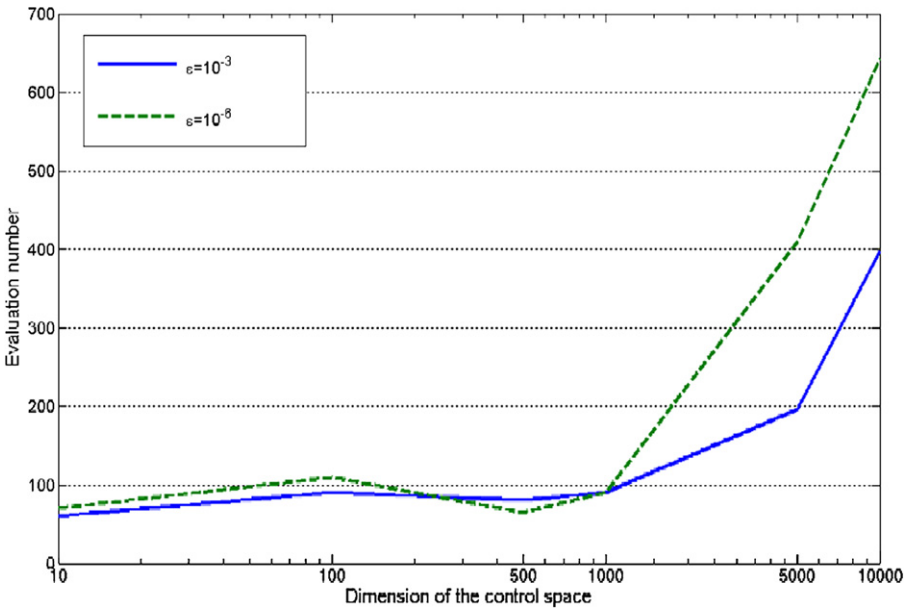

Fig. 1. Complexity evolution (number of evaluations for the pair (J, J')) in global optimization for the Rastrigin function $J(x) = N + \sum_{i=1}^N (x_i^2 - \cos(18x_i))$, $x \in [-5, 5]^N$ for two values of required accuracy $\varepsilon = 10^{-3}$ and 10^{-6}. The size N of control space ranges to 10^4. As the algorithm is semi-deterministic the values are averaged over 10 simulations, and one observes a deviation of 10 percent.

Fig. 1. Pour montrer l'efficacité de l'algorithme, nous montrons l'évolution de la complexité (i.e. nombre d'évaluations de (J, J')) pour la fonction de Rastrigin $J(x) = N + \sum_{i=1}^N (x_i^2 - \cos(18x_i))$, $x \in [-5, 5]^N$ pour deux précisions demandées $\varepsilon = 10^{-3}$ and 10^{-6} et une dimension de l'espace de contrôle N allant jusqu'à 10^4. Comme l'algorithm est semi-deterministe, ces résultats sont des moyennes sur 10 simulations et on observe une déviation de 10 pourcents.

to the stochastic feature mentioned, this is a semi-deterministic algorithm [7,6]. The algorithm is extremely efficient for cases where the functional is coercive and comes from perturbation of a convex functional. Fig. 1 shows the complexity of the algorithm for such a functional in term of the number of evaluations of the functional and its gradient for parameter spaces dimension ranging from 1 to 10 000.

4. Numerical examples

We use the MAE for the definition of a 3D surface from a given curvature. To be sure of the existence of solution, we build an inverse problem considering a target surface of the form:

$$\psi(x, y) = \left(\sum_i a_i \sin(\omega_i x)\right)\left(\sum_j b_j \sin(\omega_j y)\right) \quad \text{with } a_i, b_j, \omega_{i,j} \in \mathbb{R}.$$

We build f from this surface and try to recover the surface. Global minimization is used to solve this PDE minimizing the L^2 residual over a square calculation domain $]0, \pi[^2$. The L^2 integral is discretized on a 20×20 Cartesian mesh. We consider two one dimensional problems where $a_1 = b_1 = 1$ are frozen and one looks for $\omega_1 = \omega_1' = 1$ and 3 for the second problem. The first case corresponds to a optimal transport problem as $f > 0$. Fig. 2 shows the corresponding

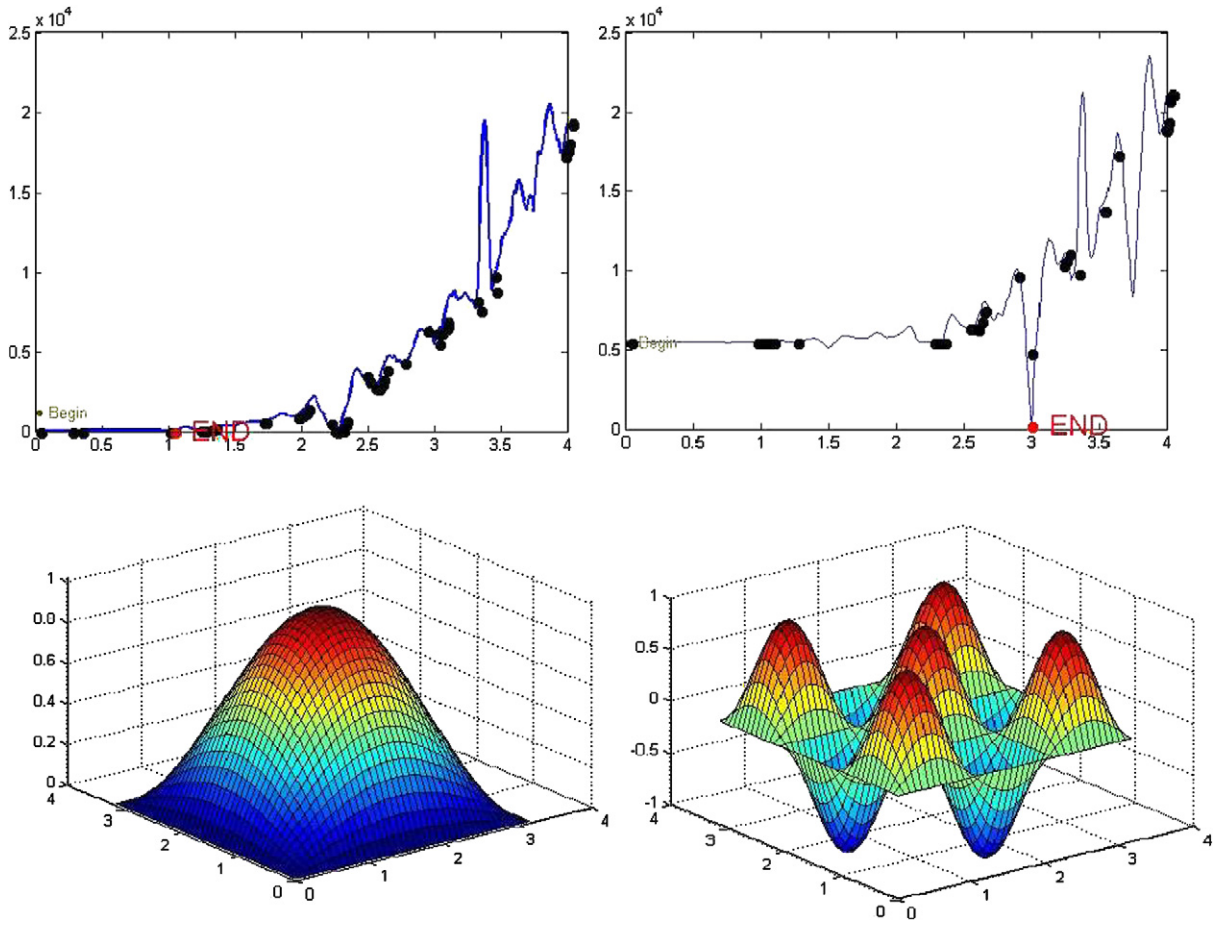

Fig. 2. Upper: typical functional for a one dimensional optimization problem obtained by sampling and the visited local minima by the global optimization approach. Lower: target surfaces solution of the Monge–Ampère equation for a strictly positive f (left) and a variable sign case (right). Both have local minima and a unique global solution.

Fig. 2. Haut : les fonctionnelles échantillonnées pour une minimisation à une dimension (gauche f positive, droite f quelconque), ainsi que les lieux visités par l'optimisation globale. Bas : surface cible pour f positive (gauche) et de signe quelconque (droite). La solution globale est unique dans les deux configurations.

functionals and surfaces. We see that both functionals have local minima and a large plateau making the minimization problem difficult.

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