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Numerical solution of the Optimal Transportation problem using the Monge–Ampère equation

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ABSTRACT

A numerical method for the solution of the elliptic Monge–Ampère Partial Differential Equation, with boundary conditions corresponding to the Optimal Transportation (OT) problem, is presented. A local representation of the OT boundary conditions is combined with a finite difference scheme for the Monge–Ampère equation. Newton's method is implemented, leading to a fast solver, comparable to solving the Laplace equation on the same grid several times. Theoretical justification for the method is given by a convergence proof in the companion paper [4]. Solutions are computed with densities supported on non-convex and disconnected domains. Computational examples demonstrate robust performance on singular solutions and fast computational times.

1. Introduction

The Optimal Transportation (OT) problem is a simply posed mathematical problem which dates back more than two centuries. It has recently led to significant results in probability, analysis, and Partial Differential Equations (PDEs), among other areas, and the subject continues to find new relevance to mathematical theory and to applications.

However, numerical solution techniques for the OT problem remain underdeveloped relative to the theory and applications. In this article we introduce a numerical method for the optimal transportation problem, which works by solving the Monge–Ampère equation, a fully nonlinear elliptic partial differential equation (PDE), with non-standard boundary conditions. We build on the foundation of the companion paper [4] to produce a new, provably convergent method for implementing the optimal transportation boundary condition for the Monge–Ampère equation. Extensive computational results demonstrate that our method correctly and efficiently solves a wide range of challenging examples.

1.1. Optimal transportation and the Monge–Ampère PDE

The OT problem is described as follows. Suppose we are given two probability densities

ρ_X, a probability density supported on X
ρ_Y, a probability density supported on Y

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where $X, Y \subset \mathbb{R}^n$ are bounded open sets and Y has to be convex. The source density ρ_X may be discontinuous and may even vanish the allowing for the support of the source density to be non-convex. The target density ρ_Y must be strictly positive and Lipschitz continuous. We discuss further in Section 1.3 the regularity and geometrical assumptions on the densities and their support.

Consider the set, $\mathbb{M}$, of maps which rearrange the measure ρ_Y into the measure ρ_X,

$$\mathbb{M} = \{T : X \mapsto Y,\ \rho_Y(T)\ \det(\nabla T) = \rho_X\}. \tag{1}$$

The OT problem, in the case of quadratic costs, is given by

$$\inf_{T \in \mathbb{M}} \frac{1}{2} \int_X \|x - T(x)\|^2 \rho_X(x)\, dx. \tag{2}$$

See Fig. 3 for an illustration of the optimal map between ellipses.

Assuming Y is convex and the densities are non-atomic, the OT problem (1), (2) is well-posed [7].

Write ∇u for the gradient, and $D^2 u$ for the Hessian, of the function u. The unique minimising map, M, at which the minimum is reached is the gradient of a convex function $u : X \subset \mathbb{R}^d \to \mathbb{R}$,

$$M = \nabla u, \quad u\,\text{convex} : X \subset \mathbb{R}^d \to \mathbb{R},$$

which is therefore also unique up to a constant. Formally substituting $T = \nabla u$ into (1) results in the Monge–Ampère PDE

$$\det\bigl(D^2 u(x)\bigr) = \frac{\rho_X(x)}{\rho_Y(\nabla u(x))}, \quad \text{for } x \in X, \tag{MA}$$

along with the restriction

$$u \text{ is convex.} \tag{C}$$

The PDE (MA) lacks standard boundary conditions. However, it is geometrically constrained by the fact that the gradient map takes X to Y,

$$\nabla u(\bar{X}) = \bar{Y}. \tag{BV2}$$

The condition (BV2) is referred to as the *second boundary value problem* for the Monge–Ampère equation in the literature (see [42]). We sometimes use the term *OT boundary conditions*.

The numerical approximation of the combined problem (MA), (BV2), (C) is the subject of this work.

1.2. Applications

The Optimal Transportation problem has applications to image registration [28], mesh generation [10], reflector design [26], astrophysics (estimating the shape of the early universe) [19], and meteorology [14], among others. See the recent textbook [44] for a discussion of the theory and a bibliography.

The OT problem also has connections with other areas of mathematics. A large class of nonlinear continuity equations with confinement and/or possibly non-local interaction potentials can be considered as semi-discrete gradient flows, known as JKO gradient flows [29,39], with respect to the Euclidean Wasserstein distance. The distance is the value function of the optimal transportation problem. The impediment so far has been the cost of numerical implementation. In one dimension the problem is trivial and [32] implements JKO gradient flow simulations for nonlinear diffusion. An interesting recent work [13] considers the two dimensional case. The performance of our solver could offer opportunities for implementing JKO gradient flows in 2D.

1.3. Weak solutions of the Monge–Ampère equation

The regularity theory for strictly convex Monge–Ampère/OT solutions is well understood and relies on the strict positivity of the densities together with the convexity of Y; see the pioneering work of Caffarelli [11] and also [44, Chapter 4]. In this framework, Brenier solutions are Alexandrov solutions and roughly speaking the potential is twice more regular than the densities functions, as one would expect for a linear second order PDE.

As explained in Section 2, the convexity of Y is an important assumption for our treatment of the boundary conditions. However, our finite difference approximation strategy will diverge from the classical regularity theory mentioned above. Our reformulation of the transport problem (MA), (BV2), (C) indeed fits within the convergence framework [8,37] of degenerate elliptic viscosity solutions [12]. This will allow for the source density ρ_X to vanish or even be discontinuous, but we require Lipschitz continuity on the target density ρ_Y.

Viscosity solutions are less general than Brenier solutions but can still capture interesting (sub)-gradient mappings. In Section 6.3 we compute the inverse mapping of the famous counter example of Caffarelli where a ball is split into a non-convex target. Because viscosity solutions allow for non-strictly convex “flat” potentials, the inverse mapping is indeed