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Machine Learning Algorithm for the Monge-Ampère Equation with Transport Boundary Conditions

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Abstract. In this article we introduce a novel numerical method to solve the problem of optimal transport and the related elliptic Monge-Ampère equation using neural networks. It is one of the few numerical algorithms capable of solving this problem efficiently with the proper transport boundary condition. Unlike the traditional deep learning solution of partial differential equations (PDEs) attributed to an optimization problem, in this paper we adopt a relaxation algorithm to split the problem into three suboptimization problems, making each subproblem easy to solve. The algorithm not only obtains the mapping that solves the optimal mass transport problem, but also can find the unique convex solution of the related elliptic Monge-Ampère equation from the mapping using deep input convex neural networks, where second-order partial derivatives can be avoided. It can be solved for high-dimensional problems, and has the additional advantage that the target domain may be non-convex. We present the method and several numerical experiments.

AMS subject classifications: 65N25, 65B99, 68T07, 65N99

Key words: Relaxation algorithm, Monge-Ampère equation, optimal transport, machine learning.

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1. Introduction

The motivation for this work is the problem of optimal mass transport. In 1781, Monge proposed a study on optimal transport (OT) when considering the best way to rearrange a pile of materials from one configuration to another. Compared to its core theories in partial differential equations (PDEs), probability, analysis are mature enough cf. [12, 41], numerical methods for the OT problem remain underdeveloped.

The optimal mass transport problem can be stated as follows. Suppose we are given two probability densities:

1) f, a probability density supported on X,

2) g, a probability density supported on Y,

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where $X, Y \subset \mathbb{R}^d$, $d \geq 2$ are bounded and compact. The problem is to find a mapping $m: X \rightarrow Y$ which minimizes the transportation cost

$$m(x) = \underset{m \in \mathbb{M}}{\operatorname{argmin}} \int_X |x - m(x)|^p f(x) dx,$$

where

$$\mathbb{M} = \left\{ m: X \rightarrow Y \;\middle|\; \int_X h\big(m(x)\big) f(x) dx = \int_Y h(p) g(p) dp \right. \\ \left. \text{for all continuous test functions } h \right\}. \tag{1.1}$$

In the original problem Monge took $p = 1$; the case $p = 2$ corresponds to the Kantorovich (or Wasserstein) distance. Same as in the most commonly studied cases, we consider the case of $p = 2$ for the remainder of this paper.

An important theorem by Brenier [5, 15] states that the unique optimal mapping is the (almost everywhere) unique gradient of a convex function, which is denoted by ∇u. By using a change of variables and coordinates, we obtain

$$\det(D^2 u) = \frac{f}{g(\nabla u)}, \tag{MA}$$

along with the restriction

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

The accompanying boundary condition is derived from the condition that m maps X to Y and reads

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

The OT problem is equivalent to Monge-Ampère equation with conditions (BV2). It is used in a wide range of fields, including computational fluid dynamics, color transfer between multiple images or deformation in the context of image processing, interpolation schemes in computer graphics, and economics, via matching and equilibrium problems. In addition, optimal transport has recently attracted the attention of biomedical-related scholars and is widely used as a data enhancement tool for guiding differentiation during single-cell RNA development as well as for improving cellular observables, thereby improving the accuracy and stability of various downstream sub-tasks. Among the many applications, we focus on mesh generation and illumination optics. In our numerical results, we will give two examples from each of these two applications.

Until now, the numerical solution of the Monge-Ampère equation is still being developed. However effective algorithms with transport conditions are still rare. An early numerical method for the related Monge-Ampère equation introduced by Oliker and Prussner [33] used a discretization based on the geometric interpretation of the solutions. Another recent method developed by Benamou *et al.* [3] introduced a new discretization wide-stencil