ARTICLE IN PRESS YJFAN:7982

Journal of Functional Analysis ••• (••••) •••–•••

Contents lists available at ScienceDirect

Journal of Functional Analysis

www.elsevier.com/locate/jfa

Unbalanced optimal transport: Dynamic and Kantorovich formulations

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ARTICLE INFO

Article history:
Received 26 January 2017
Accepted 7 March 2018
Available online xxxx
Communicated by Felix Otto

Keywords:
Unbalanced optimal transport

ABSTRACT

This article presents a new class of distances between arbitrary nonnegative Radon measures inspired by optimal transport. These distances are defined by two equivalent alternative formulations: (i) a *dynamic* formulation defining the distance as a geodesic distance over the space of measures (ii) a static "Kantorovich" formulation where the distance is the minimum of an optimization problem over pairs of couplings describing the transfer (transport, creation and destruction) of mass between two measures. Both formulations are convex optimization problems, and the ability to switch from one to the other depending on the targeted application is a crucial property of our models. Of particular interest is the Wasserstein–Fisher–Rao metric recently introduced independently by [7,15]. Defined initially through a dynamic formulation, it belongs to this class of metrics and hence automatically benefits from a static Kantorovich formulation.

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https://doi.org/10.1016/j.jfa.2018.03.008
0022-1236/

1. Introduction

Optimal transport is an optimization problem which gives rise to a popular class of metrics between probability distributions. We refer to the monograph of Villani [28] for a detailed overview of optimal transport. A major constraint of the resulting transportation metrics is that they are restricted to measures of equal total mass (e.g. probability distributions). In many applications, there is however a need to compare unnormalized measures, which corresponds to so-called *unbalanced* optimal transport problems, following the terminology introduced in [2]. Applications of these unbalanced metrics range from image classification [27,21] to the processing of neuronal activation maps [11]. This class of problems requires to precisely quantify the amount of transportation, creation and destruction of mass needed to compare arbitrary positive measures. While several proposals to achieve this goal have been made in the literature (see below for more details), to the best of our knowledge, there lacks a coherent framework that enables to deal with generic measures while preserving both the dynamic and the static perspectives of optimal transport. It is precisely the goal of the present paper to describe such a framework and to explore its main properties.

1.1. Previous work

In the last few years, there has been an increasing interest in extending optimal transport to the unbalanced setting of measures having non-equal masses.

Dynamic formulations of unbalanced optimal transport Several models based on the fluid dynamic formulation introduced in [3] have been proposed recently [19,18,22,23]. In these works, a source term is introduced in the continuity equation. They differ in the way this source is penalized or chosen. We refer to [7] for a detailed overview of these models.

Static formulations of unbalanced optimal transport Purely static formulations of unbalanced transport are however a longstanding problem. A simple way to address this issue is given in the early work of Kantorovich and Rubinstein [14]. The corresponding “Kantorovich norms” were later extended to separable metric spaces by [13]. These norms handle mass variations by allowing to drop some mass from each location with a fixed transportation cost. The computation of these norms can in fact be re-casted as an ordinary optimal transport between normalized measures by adding a point “at infinity” where mass can be sent to, as explained by [12]. This reformulation is used in [11] for applications in neuroimaging. A related approach is the so-called optimal partial transport. It was initially proposed in the computer vision literature to perform image retrieval [27, 21], while its mathematical properties are analyzed in detail by [6,9]. As noted in [7] and recalled in Section 5.1, optimal partial transport is tightly linked to the generalized transport proposed in [22,23] which allows a dynamic formulation of the optimal partial

Please cite this article in press as: L. Chizat et al., Unbalanced optimal transport: Dynamic and Kantorovich formulations, J. Funct. Anal. (2018), https://doi.org/10.1016/j.jfa.2018.03.008