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Optimal Mass Transport

Signal processing and machine-learning applications

Transport-based techniques for signal and data analysis have recently received increased interest. Given their ability to provide accurate generative models for signal intensities and other data distributions, they have been used in a variety of applications, including content-based retrieval, cancer detection, image superresolution, and statistical machine learning, to name a few, and they have been shown to produce state-of-the-art results. Moreover, the geometric characteristics of transport-related metrics have inspired new kinds of algorithms for interpreting the meaning of data distributions. Here, we provide a practical overview of the mathematical underpinnings of mass transport-related methods, including numerical implementation, as well as a review, with demonstrations, of several applications. Software accompanying this article is available from [43].

Purposes for optimal mass transport

Motivation and goals

Numerous applications in science and technology depend on effective modeling and information extraction from signal and image data. Examples include being able to distinguish between benign and malignant tumors in medical images; learning models (e.g., dictionaries) for solving inverse problems; identifying people from images of faces, voice profiles, or fingerprints; and many others. Techniques based on the mathematics of optimal mass transport, also known as *Earth Mover's Distance* in engineering-related fields, have received significant attention recently given their ability to incorporate spatial (in addition to intensity) information when comparing signals, images, and other data sources, thus giving rise to different geometric interpretations of data distributions. These techniques have been used to simplify and augment the accuracy of numerous pattern

Digital Object Identifier 10.1109/MSP.2017.2695801
Date of publication: 11 July 2017

recognition-related problems. Some examples covered in this article include image retrieval [32], [44], signal and image representation [25], [27], [40], [50], inverse problems [30], cancer detection [4], [39], texture and color modeling [18], [41], shape and image registration [22], [29], and machine learning [12], [17], [19], [28], [36], [42], to name a few. This article is meant to serve as an introductory guide to those wishing to familiarize themselves with these emerging techniques. Specifically, we

- provide a brief overview of key mathematical concepts related to optimal mass transport
- describe recent advances in transport-related methodology and theory
- provide a practical overview of their applications in modern signal analysis, modeling, and learning problems.

Why transport?

In recent years, numerous techniques for signal and image analysis have been developed to address important learning and estimation problems. Researchers working to unveil solutions to these problems have found it necessary to develop techniques to compare signal intensities across different signal/image coordinates. A common problem in medical imaging, for example, is the analysis of magnetic resonance images with the goal of learning about brain morphology differences between healthy and diseased populations. Decades of research in this area have culminated with techniques such as voxel- and deformation-based morphology that make use of nonlinear registration methods to understand differences in tissue density and locations. Likewise, the development of dynamic time-warping techniques was necessary to enable the comparison of time series data more meaningfully without confounds from commonly encountered variations in time. Furthermore, researchers desiring to create realistic models of facial appearance have long understood that appearance models for the eyes, lips, nose, and other facial features are significantly different and thus must be dependent on a position relative to a fixed anatomy. The pervasive success of these as well as other techniques, such as optical flow, level-set methods, and deep neural networks, have shown that 1) nonlinearity and 2) modeling the location of pixel intensities are essential concepts to keep in mind when solving modern regression problems related to estimation and classification.

The previously mentioned methodology for modeling appearance and learning morphology, time series analysis and predictive modeling, deep neural networks for classification of sensor data, and the like is algorithmic in nature. The transport-related techniques reviewed in this article are nonlinear methods that, unlike linear methods such as Fourier, wavelets, and dictionary models, explicitly model signal intensities and their locations. Furthermore, they are often based on the theory of optimal mass transport from which fundamental principles can be put to use. Thus, they hold the promise to ultimately play a significant role in the development of a theoretical foundation for certain subclasses of modern learning and estimation problems.

A brief historical note

The optimal mass transport problem seeks the most efficient way of transforming one distribution of mass to another, relative to a given cost function. The problem was initially studied by the French mathematician Gaspard Monge in his seminal work “Mémoire sur la Théorie des Déblais et des Remblais” [35] in 1781. In 1942, Leonid V. Kantorovich, who, at that time, was unaware of Monge’s work, proposed a general formulation of the problem by considering optimal mass transport plans, which, as opposed to Monge’s formulation, allows for mass splitting [23]. Kantorovich shared the 1975 Nobel Prize in Economic Sciences with Tjalling Koopmans for his work in the optimal allocation of scarce resources. Kantorovich’s contribution is considered “the birth of the modern formulation of optimal transport” [49], and it made the optimal mass transport problem an active field of research in the following years.

A significant portion of the theory of the optimal mass transport problem was developed in the 1990s, starting with Brenier’s seminal work on the characterization, existence, and uniqueness of optimal transport maps [9], followed by Caffarelli’s work on regularity conditions of such mappings [10] and Gangbo and McCann’s work on a geometric interpretation of the problem [20]. A more thorough history and background on the optimal mass transport problem can be found in Villani’s book *Optimal Transport: Old and New* [49] and Santambrogio’s book *Optimal Transport for Applied Mathematicians* [45]. The significant contributions in mathematical foundations of the optimal transport problem together with recent advancements in numerical methods [6], [14], [31], [37] have spurred the recent development of numerous data-analysis techniques for modern estimation and detection (e.g., classification) problems.

Formulation of the problem and methodology

While reviewing both the continuous and discrete formulations of the optimal transport problem (i.e., Monge’s and Kantorovich’s formulations), the geometrical characteristics of the problem, and the transport-based signal/image embeddings, we have elected to avoid measure-theoretic notation, and other detailed mathematical language, in lieu of a more informal and intuitive description of the problem. However, it must be said that certain mathematical precision is required to best understand the differences between Monge’s and Kantorovich’s formulation, their geometric interpretations, and other points. The interested reader may find it useful to consult [24] for a more complete and mathematical description of the concepts explained in the following sections.

Optimal transport: Formulation

Over the past century or so, the theory of optimal transport (Earth mover’s distance) has developed two main formulations, one utilizing a continuous map (Monge’s formulation) and another utilizing what is called a *transport plan* (Kantorovich’s formulation), for assigning the spatial correspondence necessary for the related transport problem. Although Monge’s

continuous formulation is helpful in problems where a point-to-point assignment is desired, Kantorovich's formulation is more general and also covers the case of discrete (Dirac) masses (in our case, signal intensities). These not only differ in mathematical formulation but also have consequences with regard to their respective numerical solutions as well as applications.

Monge's continuous formulation

The Monge optimal mass transport problem is formulated as follows. Consider two signals or images I_0 and I_1 defined over their respective domains Ω_0 and Ω_1 . Here, Ω_0 and Ω_1 are typically subsets of \mathbb{R}^d and can often be taken as the unit square (or cube in three dimensions). Although a detailed measure-theoretic formulation is typically required (see [24]), we bypass the rigorous formulation here and simply assume that $I_0(x)$ and $I_1(y)$ correspond to signal intensities at positions $x \in \Omega_0$ and $y \in \Omega_1$. For digital signals, an interpolating model can be used to construct these functions defined over continuous domains from sampled discrete data. The signals are required to be nonnegative, i.e., $I_0(x) \geq 0 \quad \forall x \in \Omega_0$ and $I_1(y) \geq 0 \quad \forall y \in \Omega_1$. In addition, the total amount of signal (or mass) for both signals should be equal to the same constant (which is generally chosen to be 1): $\int_{\Omega_0} I_0(x) dx = \int_{\Omega_1} I_1(y) dy = 1$. In other words, I_0 and I_1 are assumed to be probability density functions (PDFs).

Monge's optimal transportation problem is to find a function $f: \Omega_0 \rightarrow \Omega_1$ that pushes I_0 onto I_1 and minimizes the objective function,

$$M(I_0, I_1) = \inf_{f \in MP} \int_{\Omega_0} c(x, f(x)) I_0(x) dx, \quad (1)$$

where $c: \Omega_0 \times \Omega_1 \rightarrow \mathbb{R}^+$ is the cost of moving pixel intensity $I_0(x)$ from x to $f(x)$ [Monge considered the Euclidean distance as the cost function in his original formulation, $c(x, f(x)) = |x - f(x)|$, and *MP* stands for a measure preserving map that moves all the signal intensity from I_0 to I_1 . That is, for a subset $B \subset \Omega_1$ the MP requirement is that

$$\int_{\{x: f(x) \in B\}} I_0(x) dx = \int_B I_1(y) dy. \quad (2)$$

If f is one to one, this just means that for $A \subset \Omega_0$,

$$\int_A I_0(x) dx = \int_{f(A)} I_1(y) dy.$$

Such maps $f \in MP$ are sometimes called *transport maps* or *mass-preserving maps*. Simply put, the Monge formulation of the problem seeks to rearrange signal I_0 into signal I_1 while minimizing a specific cost function. In cases when f is smooth and one to one, then the requirement (2) can be written in a differential form as

$$\det(Df(x)) I_1(f(x)) = I_0(x) \quad (3)$$

almost everywhere, where Df is the Jacobian of f [see Figure 1(a)]. Note that both the objective function and the constraint in (1) are nonlinear with respect to $f(x)$. Hence, for

more than a century, the answers to questions regarding existence and characterization of the Monge's problem remained unknown.

For certain measures, the Monge's formulation of the optimal transport problem is ill posed in the sense that there is no transport map to rearrange one PDF to another. For instance, consider the case where I_0 is a Dirac mass and I_1 is not. Kantorovich's formulation alleviates this problem by finding the optimal transport plan as opposed to the transport map.

Kantorovich's formulation

Kantorovich formulated the transport problem by optimizing over transportation plans, which we denote as γ . One can think of γ as the joint distribution of I_0 and I_1 describing how much mass is being moved to different coordinates; i.e., let A be a subset of Ω_0 and similarly $B \subset \Omega_1$. For notational simplicity, we will not make a distinction between a probability distribution and its density. More precisely, we associate a probability distribution to a signal I_0 by $I_0(A) = \int_A I_0(x) dx$.

The quantity $\gamma(A \times B)$ tells us how much mass in set A is being moved to set B . Here, the MP constraint can be expressed as $\gamma(\Omega_0 \times B) = I_1(B)$ and $\gamma(A \times \Omega_1) = I_0(A)$. Kantorovich's formulation for the optimal transport problem can then be written as

$$K(I_0, I_1) = \min_{\gamma \in MP} \int_{\Omega_0 \times \Omega_1} c(x, y) d\gamma(x, y). \quad (4)$$

Note that the integration notation $d\gamma(x, y)$ is meant to represent the fact that this integral is more general than the routine

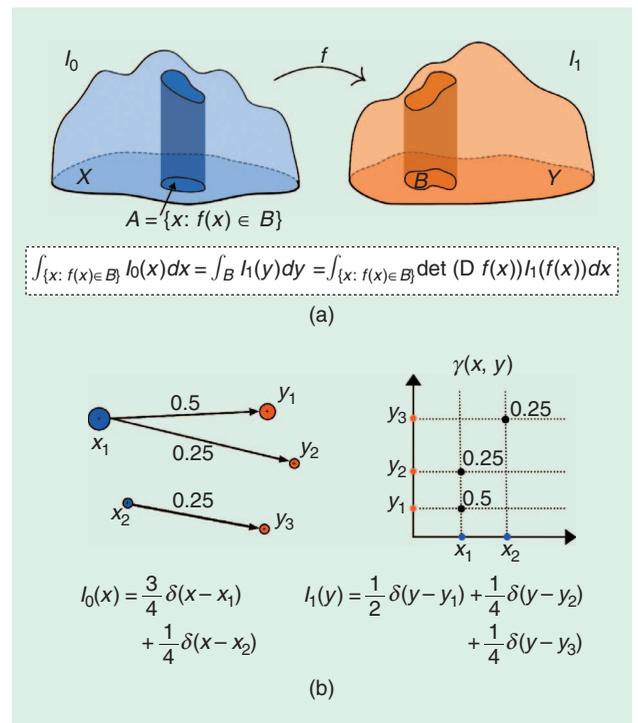


FIGURE 1. (a) The Monge transport map and (b) Kantorovich's transport plan.

Riemman-type integral commonly used in signal processing, and the integral can cover integration over domains that are more general. The minimizer of the optimization problem above, γ^* , is called the *optimal transport plan*. However, unlike the Monge problem, in Kantorovich's formulation, the objective function and the constraints are linear with respect to $\gamma(x, y)$. Moreover, Kantorovich's formulation is in the form of a convex optimization problem. We also note that the Monge problem is more restrictive than the Kantorovich problem; i.e., in Monge's version, mass from a single location in Ω_0 is being sent to a single location in Ω_1 . Kantorovich's formulation, however, considers transport plans that can deal with arbitrary measurable sets and has the ability to distribute mass from the one location in one density to multiple locations in another [see Figure 1(b)]. For any transport map $f: \Omega_0 \rightarrow \Omega_1$ there is an associated transport plan, determined by

$$\gamma(A \times B) = \int_{\{x \in A: f(x) \in B\}} I_0(x) dx. \quad (5)$$

Furthermore, when an optimal transport map f^* exists, it can be shown that the transport plan γ^* derived from (5) is an optimal transportation plan [49].

The Kantorovich problem is especially interesting in a discrete setting, i.e., for PDFs of the form $I_0 = \sum_{i=1}^M p_i \delta(x - x_i)$ and $I_1 = \sum_{j=1}^N q_j \delta(y - y_j)$, where $\delta(x)$ is the Dirac delta function. Generally speaking, for such PDFs a transport map that pushes I_0 into I_1 does not exist. In these cases, mass splitting, as allowed by the Kantorovich formulation, is necessary [see Figure 1(b)]. The Kantorovich problem can be written as

$$\begin{aligned} K(I_0, I_1) &= \min_{\gamma} \sum_i \sum_j c(x_i, y_j) \gamma_{ij} \\ \text{s.t. } \sum_j \gamma_{ij} &= p_i, \quad \sum_i \gamma_{ij} = q_j \\ \gamma_{ij} &\geq 0, \quad i = 1, \dots, M, \quad j = 1, \dots, N, \end{aligned} \quad (6)$$

where γ_{ij} identifies how much of the mass particle m_i at x_i needs to be moved to y_j [see Figure 1(b)]. The optimization above has a linear objective function and linear constraints; therefore, it is a linear programming problem. This problem is convex (which, in practice, translates to a relatively easier process of finding a global minimum), but not strictly so, and the constraint provides a polyhedral set of $M \times N$ matrices. In practice, a nondiscrete measure is often approximated by a discrete measure, and the Kantorovich problem is solved through the linear programming optimization expressed in (6).

Basic properties

Consider a transportation cost $c(x, y)$ that is continuous and bounded from below. Given two signals I_0 and I_1 as previously shown, there always exists a transportation plan minimizing (4). This holds true for both when signals I_0 and I_1 are functions and when they are discrete probability distributions [49]. Another important question is regarding the existence of an optimal transport map instead of a plan. Brenier

[9] addressed this problem for the special case where $c(x, y) = |x - y|^2$. Brenier's results were later relaxed to more general cases by Gangbo and McCann [20], which led to the following theorem.

Theorem

Let I_0 and I_1 be nonnegative functions of the same total mass and with bounded support. When $c(x, y) = h(x - y)$ for some strictly convex function h , then there exists a unique optimal transportation map f^* minimizing (1). In addition, the optimal transport plan is unique and given by (5). Moreover, if $c(x, y) = |x - y|^2$, then there exists a (unique up to adding a constant) convex function ϕ such that $f^* = \nabla\phi$. A proof is available in [20] and [49].

Optimal mass transport: Geometric properties

Wasserstein metric

Let Ω be a bounded subset of \mathbb{R}^d on which the signals are defined. As an example, for signals ($d = 1$) or images ($d = 2$), this can simply be the space $[0, 1]^d$. Let $P(\Omega)$ be the set of probability densities supported on Ω . The p -Wasserstein metric, W_p , for $p \geq 1$ on $P(\Omega)$ is then defined as using the optimal transportation problem (4) with the cost function $c(x, y) = |x - y|^p$. For I_0 and I_1 in $P(\Omega)$,

$$W_p(I_0, I_1) = \left(\inf_{\gamma \in MP} \int_{\Omega \times \Omega} |x - y|^p d\gamma(x, y) \right)^{\frac{1}{p}}.$$

For any $p \geq 1$, W_p is a metric on $P(\Omega)$. The metric space $(P(\Omega), W_p)$ is referred to as the p -Wasserstein space. To understand the nature of the optimal transportation distances, it is useful to note that for any $p \geq 1$, the convergence with respect to W_p is equivalent to the weak convergence of measures; i.e., $W_p(I_n, I) \rightarrow 0$ as $n \rightarrow \infty$ if and only if for every bounded and continuous function $f: \Omega \rightarrow \mathbb{R}$

$$\int_{\Omega} f(x) I_n(x) dx \rightarrow \int_{\Omega} f(x) I(x) dx.$$

For the specific case of $p = 1$, the p -Wasserstein metric is also known as the *Monge–Rubinstein metric* [49] or the *Earth mover's distance* [44]. The p -Wasserstein metric in one dimension has a simple characterization. For one-dimensional (1-D) signals I_0 and I_1 , the optimal transport map has a closed-form solution. Let F_i be the cumulative distribution function of I_i for $i = 0, 1$, i.e.,

$$F_i(x) = \int_{\inf(\Omega)}^x I_i(x) dx \quad \text{for } i = 0, 1.$$

Note that this is a nondecreasing function going from 0 to 1. We define the pseudoinverse of F_0 as follows: for $z \in (0, 1)$, $F_0^{-1}(z)$ is the smallest x for which $F_0(x) \geq z$, i.e.,

$$F_0^{-1}(z) = \inf \{x \in \Omega : F_0(x) \geq z\}.$$

If $I_0 > 0$, then F_0 is continuous and increasing (and thus invertible), and the inverse of the function F_0 is equal to

the pseudoinverse we just defined. In other words, the pseudoinverse is a generalization of the notion of the inverse of a function. The pseudoinverse (i.e., the inverse if $I_0 > 0$ and $I_1 > 0$) provides a closed-form solution for the p -Wasserstein distance:

$$W_p(I_0, I_1) = \left(\int_0^1 |F_0^{-1}(z) - F_1^{-1}(z)|^p dz \right)^{\frac{1}{p}}. \quad (7)$$

The closed-form solution of the p -Wasserstein distance in one dimension is an attractive property, as it alleviates the need for optimization. This property was employed in the sliced-Wasserstein metrics as defined below.

Sliced-Wasserstein metric

The idea behind the sliced-Wasserstein metric is to first obtain a set of 1-D representations for a higher-dimensional probability distribution through projections (slicing the measure) and then calculate the distance between two input distributions as a functional on the Wasserstein distance of their 1-D representations. In this sense, the distance is obtained by solving several 1-D optimal transport problems, which have closed-form solutions.

The projection of high-dimensional PDFs is closely related to the well-known Radon transform in the imaging and image processing community [8], [25]. The d -dimensional Radon transform \mathcal{R} maps a function $I \in L_1(\mathbb{R}^d)$ where $L_1(\mathbb{R}^d) := \{I: \mathbb{R}^d \rightarrow \mathbb{R} \mid \int_{\mathbb{R}^d} |I(x)| dx \leq \infty\}$ into the set of its integrals over the hyperplanes of \mathbb{R}^d . It is defined as

$$\mathcal{R}I(t, \theta) = \int_{\mathbb{R}} I(t\theta + s\theta^\perp) ds, \\ \forall t \in \mathbb{R}, \forall \theta \in \mathbb{S}^{d-1};$$

here, θ^\perp is the subspace orthogonal to θ , and \mathbb{S}^{d-1} is the unit sphere in \mathbb{R}^d . Note that $\mathcal{R}: L_1(\mathbb{R}^d) \rightarrow L_1(\mathbb{R} \times \mathbb{S}^{d-1})$. In other words, the Radon transform projects a PDF, $I \in P(\mathbb{R}^d)$, where $d > 1$, into an infinite set of 1-D PDFs $\mathcal{R}I(\cdot, \theta)$. The sliced-Wasserstein metric for PDFs I_0 and I_1 on \mathbb{R}^d is then defined as

$$SW_p(I_0, I_1) = \left(\int_{\mathbb{S}^{d-1}} W_p^p(\mathcal{R}I_0(\cdot, \theta), \mathcal{R}I_1(\cdot, \theta)) d\theta \right)^{\frac{1}{p}},$$

where $p \geq 1$, and W_p is the p -Wasserstein metric, which, for 1-D PDFs, $\mathcal{R}I_0(\cdot, \theta)$ and $\mathcal{R}I_1(\cdot, \theta)$ has a closed-form solution [see (7)]. For more details and definitions of the sliced-Wasserstein metric, we refer the reader to [8], [25] and [29].

Wasserstein spaces, geodesics, and Riemannian structure

In this section, we assume that Ω is convex. Here, we highlight that the p -Wasserstein space $(P(\Omega), W_p)$ is not just a metric space but has additional geometric structure. In particular, for any $p \geq 1$ and any $I_0, I_1 \in P(\Omega)$, there exists a continuous path (interpolation) between I_0 and I_1 whose length is the distance between I_0 and I_1 .

Furthermore, the space with $p = 2$ is special because it possesses a structure of a formal, infinite dimensional, Riemannian manifold. That structure was first noted by Otto [38], who developed the formal calculations for using this structure. The precise description of the manifold of probability measures endowed with Wasserstein metric can be found in [1].

Next, we review the two main notions that have a wide use. We characterize the geodesics in $(P(\Omega), W_p)$, and in the case of $p = 2$, we describe what is the local, Riemannian metric of $(P(\Omega), W_2)$. Finally, we state the seminal result of Benamou and Brenier [5], who provided a characterization of geodesics via action minimization, which is useful in computations and also gives an intuitive explanation of the Wasserstein metric.

We first recall the definition of the length of a curve in a metric space. Let (X, d) be a metric space and $I: [a, b] \rightarrow X$. Then the length of I , denoted by $L(I)$ is

$$L(I) = \sup_{m \in \mathbb{N}, a = t_0 < t_1 < \dots < t_m = b} \sum_{i=1}^m d(I(t_{i-1}), I(t_i)).$$

A metric space (X, d) is a geodesic space if, for any I_0 and I_1 , there exists a curve $I: [0, 1] \rightarrow X$ such that $I(0) = I_0$, $I(1) = I_1$ and for all $0 \leq s < t \leq 1$, $d(I(s), I(t)) = L(I|_{[s,t]})$. In particular, the length of I is equal to the distance from I_0 to I_1 . Such a curve I is called a *geodesic*. The existence of geodesics is useful because it allows one to define the average of I_0 and I_1 as the midpoint of the geodesic connection between them.

An important property of $(P(\Omega), W_p)$ is that it is a geodesic space and that geodesics are easy to characterize. Specifically, they are given by the displacement interpolation (also known as a *McCann interpolation*). When a unique transportation map f^* from I_0 to I_1 exists that minimizes (1) for $c(x, y) = |x - y|^p$, the geodesic is obtained by moving the mass at constant speed from x to $f^*(x)$. More precisely, for $t \in [0, 1]$ and $x \in \Omega$ let

$$f_t^*(x) = (1 - t)x + tf^*(x)$$

be the position at time t of the mass initially at x . Note that f_0^* is identity mapping and $f_1^* = f^*$. Pushing forward the mass by f_t^* , which by (3) has the form

$$I_t(f_t^*(x)) = \frac{I_0(x)}{\det(Df_t^*(x))}$$

if f^* is smooth, provides the desired geodesic from I_0 to I_1 . The velocity of each particle $\partial_t f_t^* = f^*(x) - x$ is the displacement of the optimal transportation map. Figure 2 conceptualizes the geodesic between two PDFs in $P(\Omega)$ and visualizes it for three different pairs of PDFs.

An important fact regarding the 2-Wasserstein space is Otto's presentation of a formal Riemannian metric for this space [38]. It involves shifting to a Lagrangian point of view. To explain, consider the path $I(x, t)$ in $P(\Omega)$ with $I(x, t)$ smooth. Then $s(x, t) = \partial I / \partial t(x, t)$ can be considered a tangent vector to the manifold or a density perturbation. Instead of thinking

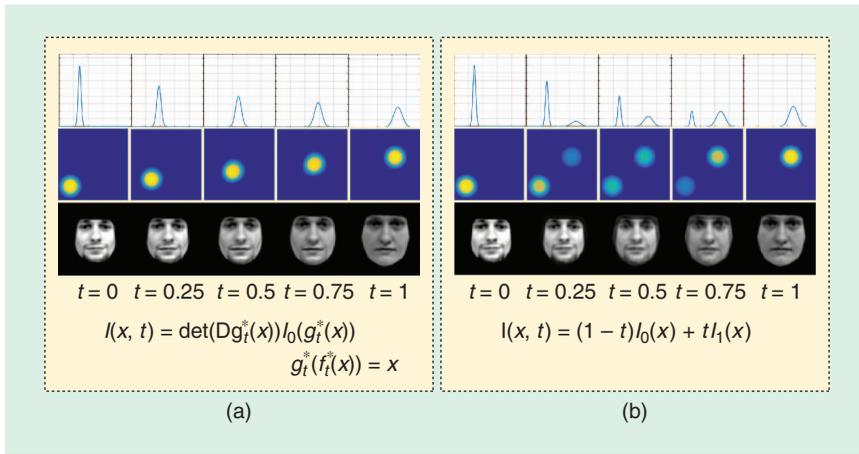


FIGURE 2. Geodesics in (a) the 2-Wasserstein space and in (b) the Euclidean space between various 1-D and two-dimensional (2-D) PDFs. Note that the geodesic in the 2-Wasserstein space captures the nonlinear structure of the signals and images and provides a natural morphing. (Face portraits courtesy of the public CMU Pose, Illumination, and Expression database.)

of increasing/decreasing the density, this perturbation can be viewed as resulting from moving the mass by a vector field. In other words, consider vector fields $v(x, t)$ such that

$$s = -\nabla \cdot (Iv). \quad (8)$$

There are many such vector fields. Otto defined the size of $s(\cdot, t)$ as the square root of the minimal kinetic energy of the vector field that produces the perturbation to density s , i.e.,

$$\langle s, s \rangle = \min_{v \text{ satisfies (8)}} \int |v|^2 I dx. \quad (9)$$

Utilizing the Riemmanian manifold structure of $P(\Omega)$ together with the inner product presented in (9), the 2-Wasserstein metric can be reformulated into finding the minimizer of the following action among all curves in $P(\Omega)$ connecting I_0 and I_1 [5],

$$\begin{aligned} W_2^2(I_0, I_1) &= \inf_{I, v} \int_0^1 \int_{\Omega} I(x, t) |v(x, t)|^2 dx dt \\ \text{s.t. } &\partial_t I + \nabla \cdot (Iv) = 0 \\ &I(\cdot, 0) = I_0(\cdot), I(\cdot, 1) = I_1(\cdot), \end{aligned}$$

where the first constraint is the well-known continuity equation.

Optimal transport: Embeddings and transforms

The optimal transport problem and, specifically, the 2-Wasserstein metric and the sliced-2-Wasserstein metric have been recently used to define nonlinear transforms for signals and images [25], [27], [40], [50]. In contrast to commonly used linear signal transformation frameworks (e.g., Fourier and wavelet transforms) that employ signal intensities only at fixed coordinate points, thus adopting an Eulerian point of view, the idea behind transport-based transforms is to consider the intensity variations together with the locations of the intensity variations in the signal. Therefore, such

transforms adopt a Lagrangian point of view for analyzing signals; i.e., they are able to move signal (pixel) intensities around. Moreover, the transforms can be viewed as Euclidean embeddings for the data, under the previously described transport-related metric space structure. The benefit of such a Euclidean embedding is that they facilitate the application of many standard data-analysis algorithms (e.g., learning). Here, we briefly describe these transforms and some of their prominent properties.

The linear optimal transportation framework

The linear optimal transportation (LOT) framework was proposed by Wang et al.

[50]. The framework was used in [4] and [39] for pattern recognition in biomedical images and specifically histopathology and cytology images. Later, it was extended in [27] as a generic framework for pattern recognition, and it was used in [26] for the single-frame superresolution reconstruction of face images. The LOT framework, which provides an invertible Lagrangian transform for images, was initially proposed as a method to simultaneously amend the computationally expensive requirement of calculating pairwise 2-Wasserstein distance between N signals for pattern recognition purposes and to allow for the construction of generative models for images involving textures and shapes. For a given set of images $I_i \in P_2(\Omega)$, for $i = 1, \dots, N$, and a fixed template I_0 , all non-negative and having been normalized to have the same sum, the transform projects the images to the tangent space at I_0 . The projections are acquired by finding the optimal velocity fields corresponding to the optimal transport plans between I_0 and each image in the set.

The framework provides a linear embedding for $P_2(\Omega)$ with respect to a fixed signal $I_0 \in P_2(\Omega)$. This means that the Euclidean distance between an embedded signal, denoted as \tilde{I}_i , and the fixed reference, I_0 , is equal to $W_2(I_0, I_i)$, and the Euclidean distance between two embedded normalized signals is, generally speaking, an approximation of their 2-Wasserstein distance. The geometric interpretation of the LOT framework is presented in Figure 3. The linear embedding then facilitates the application of linear techniques such as principal component analysis (PCA) and linear discriminant analysis (LDA) to probability measures.

The cumulative distribution transform

Park et al. [40] considered the LOT framework for 1-D PDFs (positive signals normalized to integrate to 1), and since in dimension one the transport maps are explicit, they were able to characterize the properties of the transformed densities. Similar to the LOT framework, let I_i for $i = 1, \dots, N$ and I_0 be signals (PDFs) defined on \mathbb{R} . The framework first

calculates the optimal transport maps between I_i and I_0 using $f_i(x) = F_i^{-1} \circ F_0(x)$ for all $i = 1, \dots, N$. Then the forward and inverse transport-based transform, denoted as the cumulative distribution transform (CDT) by Park et al. [40], for these density functions with respect to the fixed template I_0 is defined as

$$\begin{cases} \tilde{I}_i = (f_i - Id)\sqrt{I_0} & \text{(Analysis)} \\ I_i = (f_i^{-1})'(I_0 \circ f_i^{-1}) & \text{(Synthesis)} \end{cases}$$

where $(I_0 \circ f_i^{-1})(x) = I_0(f_i^{-1}(x))$. Note that the L_2 -norm (Euclidean distance) of the transformed signals, \tilde{I}_i , corresponds to the 2-Wasserstein distance between I_0 and I_i . In contrast to the higher-dimensional LOT, however, the Euclidean distance between two transformed (embedded) signals \tilde{I}_i and \tilde{I}_j , is the exact 2-Wasserstein distance between I_i and I_j (see [40] for a proof) and not just an approximation. Hence, the transformation is isometric (preserves) with respect to the 2-Wasserstein metric. This isometric nature of the CDT was utilized in [28] to provide positive definite kernels for machine learning of n -dimensional signals.

From a signal processing point of view, the CDT is a non-linear signal transformation that captures certain nonlinear variations in signals including translation and scaling. Specifically, it gives rise to the transformation pairs presented in Table 1. From Table 1, one can observe that although $I(t - \tau)$ is non-linear in τ (when $I(\cdot)$ is not a linear function), its CDT representation $\tilde{I}(t) + \tau\sqrt{I_0(t)}$ becomes affine in τ (a similar effect is observed for scaling). In effect, the Lagrangian transformations (compositions) in original signal space are rendered into Eulerian perturbations in transform space, borrowing from the partial differential equation (PDE) parlance. Furthermore, Park et al. [40] demonstrated that the CDT facilitates certain pattern recognition problems. More precisely, the transformation turns certain not linearly separable and disjoint classes of signals into linearly separable ones. Formally, let C be a set of 1-D maps, and let $P, Q \subset P_2(\Omega)$ be sets of positive PDFs born from two positive PDFs $p_0, q_0 \in P_2(\Omega)$ (which we denote as mother density functions or signals) as

$$\begin{aligned} P &= \{p \mid p = h'(p_0 \circ h), \forall h \in C\}, \\ Q &= \{q \mid q = h'(q_0 \circ h), \forall h \in C\}. \end{aligned}$$

If there exists no $h \in C$ for which $p_0 = h'(q_0 \circ h)$, then the sets P and Q are disjoint but not necessarily linearly separable in the signal space. A main result of [40] states that the signal classes P and Q are guaranteed to be linearly separable in the transform space (regardless of the choice of the reference signal I_0) if C satisfies the following conditions:

- 1) $h \in C \Rightarrow h^{-1} \in C$
- 2) $h_1, h_2 \in C \Rightarrow \rho h_1 + (1 - \rho)h_2 \in C, \forall \rho \in [0, 1]$
- 3) $h_1, h_2 \in C \Rightarrow h_1(h_2), h_2(h_1) \in C$
- 4) $h'(p_0 \circ h) \neq q_0, \forall h \in C$.

The set of translations $C = \{f \mid f(x) = x + \tau, \tau \in \mathbb{R}\}$ and scaling $C = \{f \mid f(x) = ax, a \in \mathbb{R}^+\}$, for instance, satisfy the

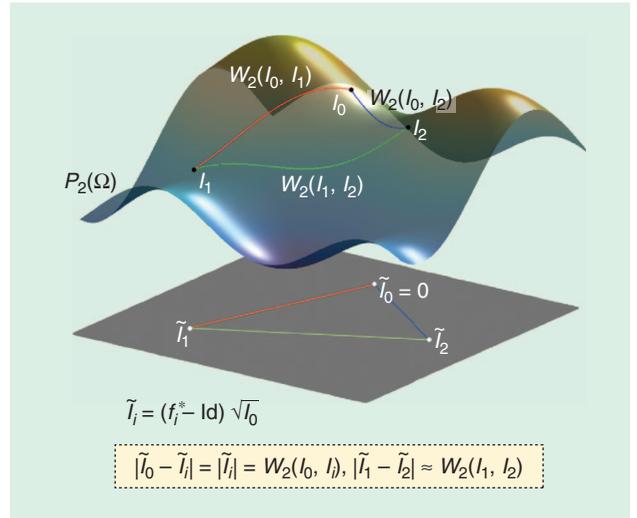


FIGURE 3. A graphical representation of the LOT framework. The framework embeds the PDFs (i.e., signals or images) I_i in the tangent space (i.e., the set of all tangent vectors) of $P_2(\Omega)$ with respect to a fixed PDF I_0 . As a consequence, the Euclidean distance between the embedded functions \tilde{I}_i and \tilde{I}_j provides an approximation for the 2-Wasserstein distance, $W_2(I_i, I_j)$.

above conditions. We refer the reader to [40] for further information. Figure 4(a) and (b) demonstrates the linear separation property of the CDT. The signal classes P and Q are chosen to be the set of all translations of a single Gaussian and a Gaussian mixture including two Gaussian functions with a fixed mean difference, respectively. The discriminant subspace is calculated for these classes, and it is shown that although the signal classes are not linearly separable in the signal domain, they become linearly separable in the transform domain.

The Radon CDT

The CDT framework was extended to 2-D density functions (images) through the sliced-Wasserstein distance in [25] and was denoted the Radon CDT. It is shown in [25] that similar characteristics of the CDT, including the linear separation property, also hold for the Radon CDT. Figure 4 clarifies the linear separation property of the Radon CDT and demonstrate the capability of such transformations. In particular, Figure 4(c) and (d) shows a facial expression data set with two classes (i.e., neutral and smiling expressions) and its corresponding representations in the LDA discriminant subspace calculated from the images [Figure 4(c)] and the Radon CDT of the data set

Table 1. The CDT pairs. Note that the composition holds for all strictly monotonically increasing functions g .

Property	Signal Domain $I(x)$	CDT Domain $\tilde{I}(x)$
Translation	$I(x - \tau)$	$\tilde{I}(x) + \tau\sqrt{I_0(x)}$
Scaling	$aI(ax)$	$\frac{\tilde{I}(x)}{a} - x\frac{(a-1)}{a}\sqrt{I_0(x)}$
Composition	$g'(x)I(g(x))$	$(g^{-1}(\frac{\tilde{I}(x)}{\sqrt{I_0(x)}}) + x) - x\sqrt{I_0(x)}$

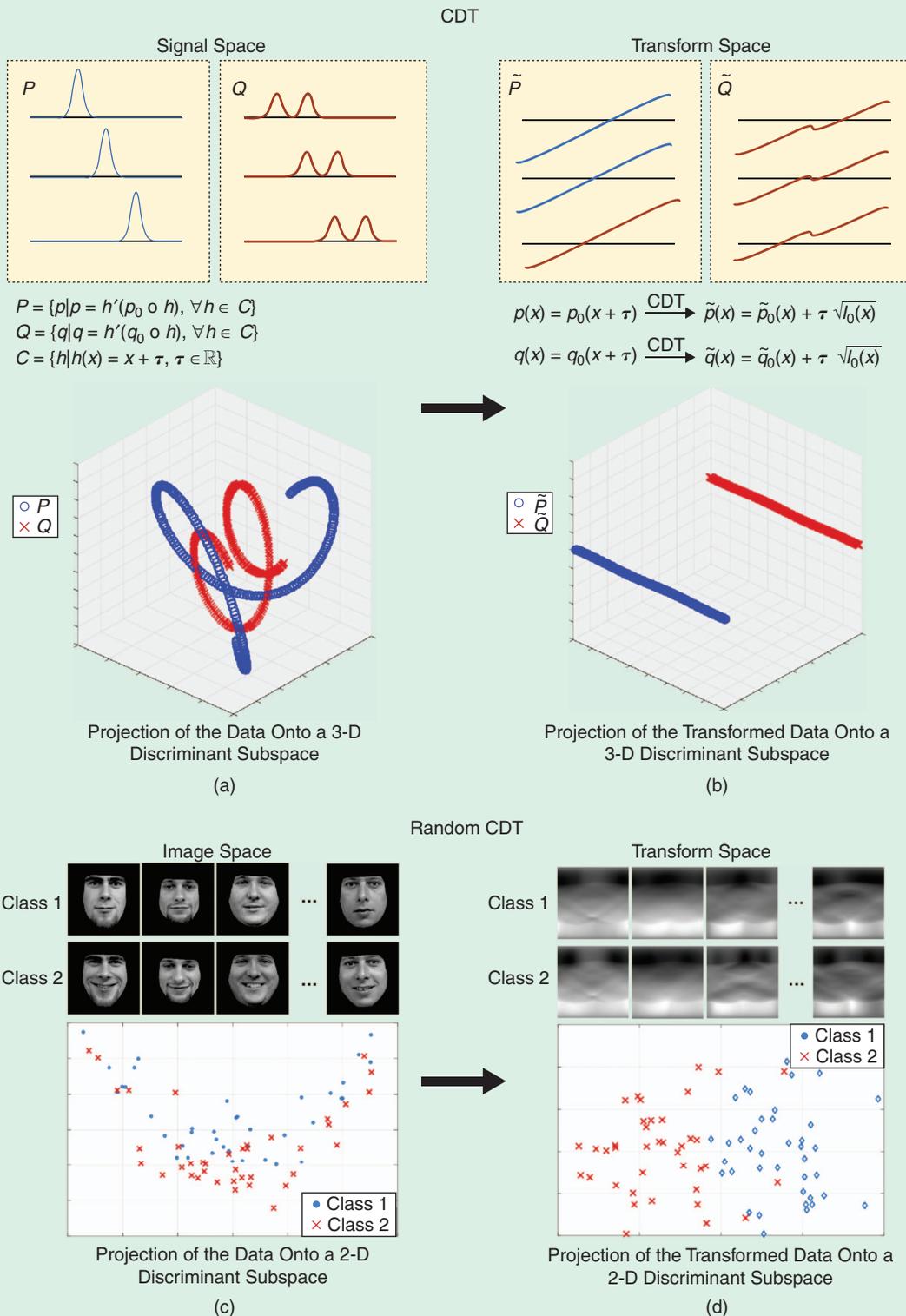


FIGURE 4. Examples for the linear separability characteristic of the CDT and the Radon CDT. The discriminant subspace for each case is calculated using the penalized-linear discriminant analysis. It can be seen that the nonlinear structure of the data is well captured in the transform spaces. (a) and (b) The linear separation property of the CDT. (c) A facial expression data set with two classes and its corresponding representations in the LDA discriminant subspace and (d) the Radon CDT of the data set and the corresponding representation of the transformed data in the LDA discriminant subspace. 3-D: three-dimensional. (Face portraits courtesy of the public CMU Pose, Illumination, and Expression database.)

and the corresponding representation of the transformed data in the LDA discriminant subspace [Figure 4(d)]. It is clear that the image classes become more linearly separable in the transform space. In addition, the cumulative percentage variation (CPV) of the data set in the image space, the Radon transform space, the Ridgelet transform space, and the Radon-CDT space are shown in Figure 5. The figure shows that the variations in the data set could be explained with fewer components in the Radon-CDT space.

Numerical methods

The development of robust and efficient numerical methods for computing transport-related maps, plans, metrics, and geodesics is crucial for the development of algorithms that can be used in practical applications. We next present several notable approaches for finding transportation maps and plans. Table 2 provides a high-level overview of these methods.

A linear programming problem

The linear programming problem is an optimization problem with a linear objective function and linear equality and inequality constraints. Several numerical methods exist for solving linear programming problems, among which are the simplex method and its variations and the interior-point methods. The computational complexity of the mentioned numerical methods, however, scales at best cubically in the size of the domain. Hence, assuming the measures considered have N particles, the number of unknowns γ_{ij} s is N^2 and the computational complexities of the solvers are at best $\mathcal{O}(N^3 \log N)$ [14], [44]. The computational complexity of the linear programming methods is a very important limiting factor for the applications of the Kantorovich problem.

We note that, in the special case where I_0 and I_1 both have N equidistributed particles, the optimal transport problem

simplifies to a one-to-one assignment problem that can be solved in $\mathcal{O}(N^2 \log N)$. In addition, several multiscale approaches and sparse approximation approaches have recently been introduced to improve the computational performance of the linear programming solvers [37], [46].

Entropy-regularized solution

Cuturi's work [14] provides a fast and easy-to-implement variation of the Kantorovich problem by considering the transportation problem from a maximum-entropy perspective. The idea is to regularize the Wasserstein metric by the entropy of the transport plan. This modification simplifies the problem and enables much faster numerical schemes with complexity

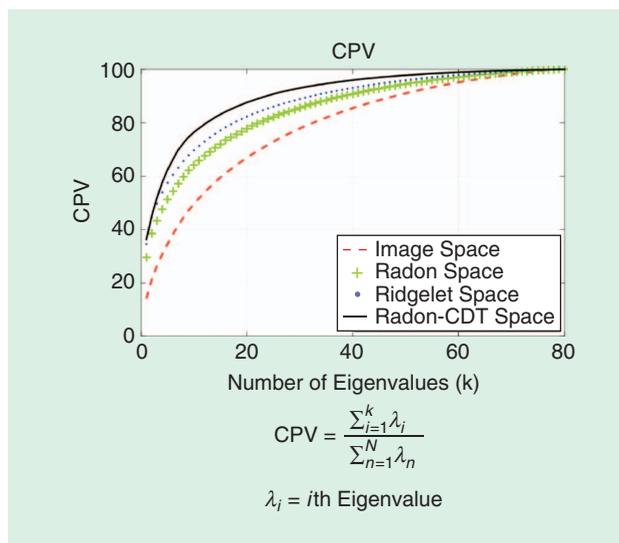


FIGURE 5. The cumulative percentage of the face data set in Figure 4 in the image space, the Radon transform space, the Ridgelet transform space, and the Radon-CDT transform space.

Table 2. The key properties of various numerical approaches.

Comparison of Numerical Approaches

Method	Remark
Linear programming	Applicable to general costs. Good approach if the PDFs are supported at very few sites.
Multiscale linear programming	Applicable to general costs. Fast and robust method, though truncation involved can lead to imprecise distances.
Auction algorithm	Applicable only when the number of particles in the source and the target is equal and all of their masses are the same.
Entropy-regularized linear programming	Applicable to general costs. Simple and performs very well in practice for moderately large problems. Difficult to obtain high accuracy.
Fluid mechanics	This approach can be adapted to generalizations of the quadratic cost, based on action along paths.
AHT minimization	Quadratic cost. Requires some smoothness and positivity of densities. Convergence is guaranteed only for infinitesimal step size.
Gradient descent on the dual problem	Quadratic cost. Convergence depends on the smoothness of the densities, hence a multiscale approach is needed for nonsmooth densities (i.e., normalized images).
Monge–Ampère solver	Quadratic cost. One in [7] is proved to be convergent. Accuracy is an issue due to the wide stencil used.
Semidiscrete approximation	An efficient way to find the map between a continuous and discrete signal [31].

AHT: Angenent, Haker, and Tannenbaum.

$O(N^2)$ [14] or $O(N \log(N))$ using the convolutional Wasserstein distance presented in [47] (compared to $O(N^3)$ of the linear programming methods), where N is the number of delta masses in each of the measures. The disadvantage is that it is difficult to obtain high-accuracy approximations of the optimal transport plan. The entropy-regularized p -Wasserstein distance, also known as the *Sinkhorn distance*, between PDFs I_0 and I_1 defined on the metric space (Ω, d) is defined as

$$W_{p,\lambda}^p(I_0, I_1) = \inf_{\gamma \in MP} \int_{\Omega \times \Omega} d^p(x, y) \gamma(x, y) dx dy + \lambda \int_{\Omega \times \Omega} \gamma(x, y) \ln(\gamma(x, y)) dx dy, \quad (10)$$

where the regularizer is the negative entropy of the plan. We note that this is not a true metric since $W_{p,\lambda}^p(I_0, I_1) > 0$. Since the entropy term is strictly concave, the overall optimization in (10) becomes strictly convex. It is shown in [14] that the entropy-regularized p -Wasserstein distance in (10) can be reformulated as

$$W_{p,\lambda}^p(I_0, I_1) = \lambda^* \inf_{\gamma \in MP} KL(\gamma | \mathcal{K}_\lambda),$$

where $\mathcal{K}_\lambda(x, y) = \exp(-d^p(x, y)/\lambda)$ and $KL(\gamma | \mathcal{K}_\lambda)$ is the Kullback–Leibler (KL) divergence between γ and \mathcal{K}_λ . In short, the regularizer enforces the plan to be within $1/\lambda$ radius in the KL-divergence sense from the transport plan $\gamma^*(x, y) = I_0(x)I_1(y)$.

Cuturi shows that the optimal transport plan γ in (10) is of the form $D_v \mathcal{K}_\lambda D_w$, where D_v and D_w are diagonal matrices with diagonal entries $v, w \in \mathbb{R}^N$ [14]; therefore, the number of unknowns in the regularized formulation is reduced from N^2 to $2N$. The new problem can then be solved through computationally efficient algorithms such as the iterative proportional fitting procedure, also known as the *iterative proportional fitting procedure algorithm*, or, alternatively, through the Sinkhorn–Knopp algorithm.

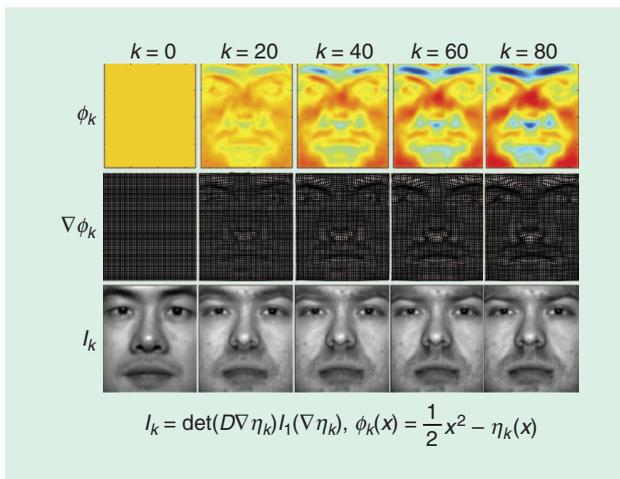


FIGURE 6. A visualization of the iterative update of the transport potential and correspondingly the transport displacement map through CWVB iterations. (Face portraits courtesy of the public Extended Yale Face Database B.)

Flow minimization (AHT)

Angenent, Haker, and Tannenbaum [2], proposed a flow minimization scheme to obtain the optimal transport map from the Monge problem. The method was used in several image-registration applications [22], pattern recognition [27], [50], and computer vision [26]. A brief review of the method is provided here.

Let $I_0: X \rightarrow \mathbb{R}^+$ and $I_1: Y \rightarrow \mathbb{R}^+$ be continuous probability densities defined on convex domains $X, Y \subseteq \mathbb{R}^d$. To find the optimal transport map, f^* , AHT starts with an initial transport map, $f_0: X \rightarrow Y$ calculated from the Knothe–Rosenblatt coupling [49]. Then it updates f_0 to minimize the transport cost while constraining it to remain a transport map from I_0 to I_1 . The updated equation for finding the optimal transport map in AHT is calculated to be

$$f_{k+1}(x) = f_k(x) + \epsilon \frac{1}{I_0} Df_k(f_k - \nabla(\Delta^{-1} \text{div}(f_k))),$$

where ϵ is the step size, Df_k is the Jacobian matrix, and Δ^{-1} is the Poisson solver with Neumann boundary conditions. AHT show that for infinitesimal step size, ϵ , $f_k(x)$ converges to the optimal transport map. For a detailed derivation of the preceding equation, see [2] and [24].

The AHT method is, in essence, a gradient descent method on the Monge formulation of the optimal transport problem. Chartrand, Wohlberg, Vixie, and Boltt (CWVB) [11] proposed an alternative gradient-descent method based on Kantorovich’s dual formulation of the transport problem that updates the optimal potential transport field, $\eta(x)$, where $f(x) = \nabla \eta(x)$. Figure 6 presents the iterations of the CWVB method for two face images taken from the YaleB face database.

Monge–Ampère equation

The Monge–Ampère PDE is defined as

$$\det(H\phi) = h(x, \phi, D\phi)$$

for some functional h and where $H\phi$ is the Hessian matrix of ϕ . The Monge–Ampère PDE is closely related to the Monge problem for the quadratic cost function. According to Bernier’s theorem (discussed in the “Basic Properties” section), when I_0 and I_1 are absolutely continuous PDFs defined on sets $X, Y \subseteq \mathbb{R}^n$, the optimal transport map that minimizes the 2-Wasserstein metric is uniquely characterized as the gradient of a convex function $\phi: X \rightarrow Y$. Moreover, we showed that the mass-preserving constraint of the Monge problem can be written as $\det(Df)I_1(f) = I_0$. Combining these results, one can have

$$\det(D(\nabla \phi(x))) = \frac{I_0(x)}{I_1(\nabla \phi)}, \quad (11)$$

where $D\nabla \phi = H\phi$, and, therefore, the equation shown above is in the form of the Monge–Ampère PDE. Now, if ϕ is a convex function on X satisfying $\nabla \phi(X) = Y$ and solving (11), then $f^* = \nabla \phi$ is the optimal transportation map from I_0 to I_1 .

The geometrical constraint on this problem is rather unusual in PDEs and is often referred to as the *optimal transport boundary conditions*. Several authors have proposed numerical methods to obtain the optimal transport map through solving the Monge–Ampère PDE in (11) [7], [33]. In particular, the scheme in [7] is monotone, has complexity $O(N)$ (up to logarithms), and is provably convergent. We conclude by remarking that several regularity results on the optimal transport maps were established through the Monge–Ampère equation (see [24] for references).

Semidiscrete approximation

Several works [31], [34] have considered the problem in which one PDF, I_0 , has a continuous form while the other, I_1 is discrete, $I_1(y) = \sum q_i \delta(y - y_i)$. It turns out there exist weights w_i such that the optimal transport map $f: X \rightarrow Y$ can be described via a power diagram. More precisely, the set of x mapping to y_i is the following cell of the power diagram:

$$PD_w(y_i) = \{x: |x - y_i|^2 - w_i \leq |x - y_j|^2 - w_j, \forall j\}.$$

The main observation is that the weights w_i are minimizers of the following unconstrained convex functional:

$$\sum_i \left(q_i w_i - \int_{PD_w(y_i)} (||x - y_i||^2 - w_i) I_0(x) dx \right).$$

Works by Mérigot [34] and Levy [31] use Newton-based schemes and multiscale approaches to minimize the functional. The need to integrate over the power diagram makes the implementation somewhat geometrically delicate. Nevertheless, a recent implementation by Levy [31] gives impressive results in terms of speed. This approach provides the transportation mapping (not just the approximation of a plan).

Applications

Image retrieval

One of the earliest applications of the optimal transport problem was in image retrieval. Rubner et al. [44] employed the discrete Wasserstein metric, which they denoted the Earth mover’s distance, to measure the dissimilarity between image signatures. In image-retrieval applications, it is common practice first to extract features (i.e., color features, texture feature, shape features, and so on) and then generate high-dimensional histograms or signatures (histograms with dynamic/adaptive binning) to represent images. The retrieval task then simplifies to finding images with similar representations (e.g., small distance between their histograms/signatures). The Wasserstein metric is specifically suitable for such applications because it can compare histograms/signatures of different sizes (histograms with different binning). This unique capability turns the Wasserstein metric into an attractive candidate in image-retrieval applications [32], [44]. In [44], the Wasserstein metric was compared with common metrics such as Jeffrey’s divergence, the χ^2 statistic, the L_1 distance, and the L_2 distance in an

image-retrieval task, and it was shown that the Wasserstein metric achieves the highest precision/recall performance among all.

Speed of computation is an important practical consideration in image-retrieval applications. For almost a decade, the high computational cost of the optimal transport problem overshadowed its practicality in large-scale image-retrieval applications. Recent advancements in numerical methods, including the work of Merigot [34] and Cuturi [14], among many others, have reinvigorated optimal transport-based distances as a feasible and appealing candidate for large-scale image-retrieval problems.

Registration and morphing

Image registration deals with finding a common geometric reference frame between two or more images. It plays an important role in analyzing images obtained at different times or using different imaging modalities. Image registration and, more specifically, biomedical image registration are active areas of research. Registration methods find a transformation f that maximizes the similarity between two or more image representations (e.g., image intensities and image features). Among the plethora of registration methods, nonrigid registration methods are especially important given their numerous applications in biomedical problems. They can be used to quantify the morphology of different organs, correct for physiological motion, and allow for comparison of image intensities in a fixed coordinate space (atlas). Generally speaking, nonrigid registration is a nonconvex and nonsymmetric problem, with no guarantee of the existence of a globally optimal transformation.

Various works in the literature deploy the Monge problem for image warping and elastic registration. Utilizing the Monge problem in an image-warping/registration setting has a number of advantages. First, the existence and uniqueness of the global transformation (the optimal transport map) is known. Second, the problem is symmetric, meaning that the optimal transport map for warping I_0 to I_1 is the inverse of the optimal transport map for warping I_1 to I_0 . Last, it provides a landmark-free and parameter-free registration scheme with a built-in mass preservation constraint. These advantages motivated several follow-up works to investigate the application of the Monge problem in image registration and warping [21], [22].

In addition to images, the optimal mass transport problem has also been used in point cloud and mesh registration [29] (see [24] for more references), which have various applications in shape analysis and graphics. In these applications, shape images (2-D or 3-D binary images) are first represented using either sets of weighted points (e.g., point clouds), using clustering techniques such as K-means or fuzzy C-means, or with meshes. Then a regularized variation of the optimal transport problem is solved to match such representations. The regularization on the transportation problem is often imposed to enforce the neighboring points (or vertices) to remain near each other after the transformation.

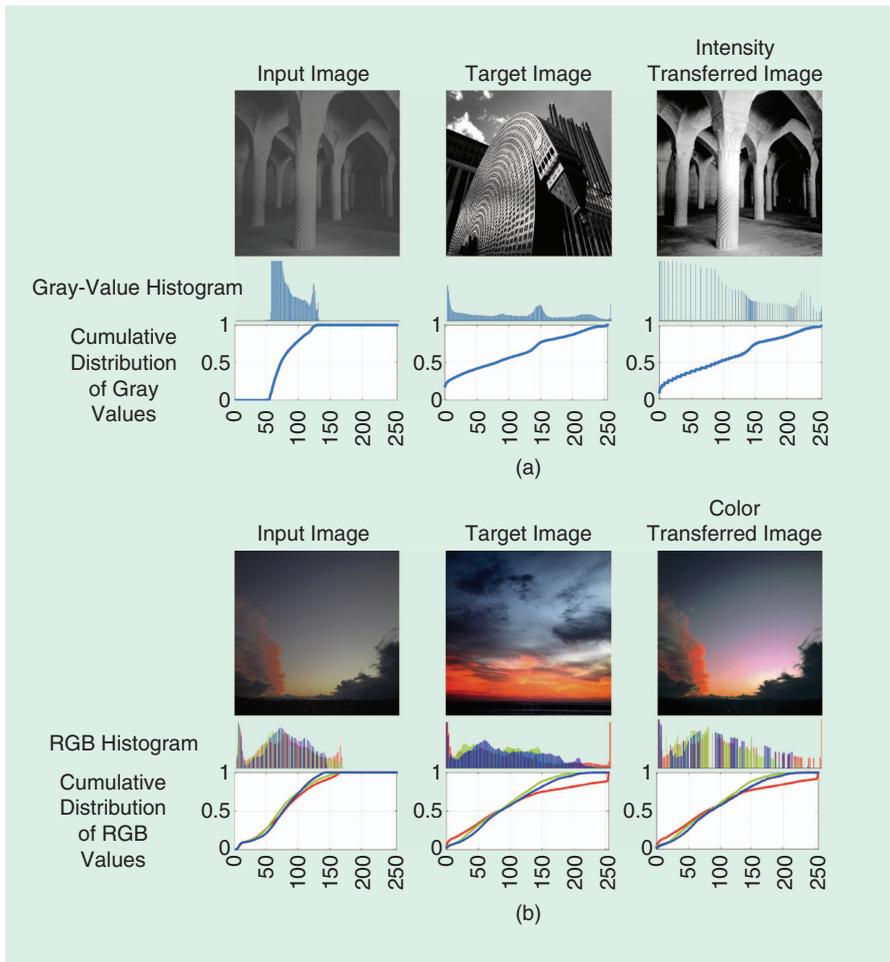


FIGURE 7. (a) Gray value and (b) color transfer via optimal transportation. RGB: red, green, blue.

Color transfer and texture synthesis

Texture mixing and color transfer are appealing applications of the optimal transport framework in image analysis, graphics, and computer vision. Here, we briefly discuss these applications.

Color transfer

The purpose of color transfer is to change the color palette of an image to impose the feel and look of another image. Color transfer is generally performed through finding a map, which morphs the color distribution of the first image into the second one. For grayscale images, the color-transfer problem simplifies to a histogram-matching problem, which is solved through the 1-D optimal transport formulation [16]. In fact, the classic problem of histogram equalization is a 1-D transport problem [16]. The color-transfer problem, on the other hand, is concerned with pushing the 3-D color distribution of the first image into the second one. This problem can also be formulated as an optimal transport problem, as demonstrated in [41] (see [24] for more references).

A complication that occurs in the color transfer on real images, however, is that a perfect match between color dis-

tributions of the images is often not satisfying, because a color-transfer map may not transfer the colors of neighboring pixels in a coherent manner and may introduce artifacts in the color-transferred image. Therefore, the color-transfer map is often regularized to make the transfer map spatially coherent [41]. Figure 7 shows a simple example of gray-value and color transfer via the optimal transport framework. It can be seen that the cumulative distribution of the gray-value and color-transferred images are similar to that of the input image.

Texture synthesis and mixing

Texture synthesis is the problem of synthesizing a texture image that is visually similar to an exemplar input-texture image and has various applications in computer graphics and image processing. Many methods have been proposed for texture synthesis, such as synthesis by recopy and synthesis by statistical modeling. Texture mixing, however, considers the problem of synthesizing a texture image from a collection of input-texture images in a way that the synthesized texture provides a meaningful integra-

tion of the colors and textures of the input-texture images. Metamorphosis is one of the successful approaches in texture mixing; it performs the mixing via identifying correspondences between elementary features (i.e., textons) among input textures and progressively morphing between the shapes of elements. In other approaches, texture images are first parametrized through a tight frame (often steerable wavelets), and statistical modeling is performed on the parameters.

Other successful approaches include random phase and spot noise texture modeling [18], which model textures as stationary Gaussian random fields. These models are based on the assumption that the visual texture perception is based on the spectral magnitude of the texture image. Therefore, utilizing the spectral magnitude of an input image and randomizing its phase will lead to a new synthetic texture image that is visually similar to the input image. Ferradans et al. [18] utilized this assumption together with the Wasserstein geodesics to interpolate between spectral magnitude of texture images and provide synthetic mixed texture images. Figure 8 shows an example of texture missing via the Wasserstein geodesic between the spectral magnitudes of the input-texture images. The in-between images are synthetically generated using the random-phase technique.

Image denoising and restoration

The optimal transport problem has also been used in several image-denoising and -restoration problems [30]. The goal in these applications is to restore or reconstruct an image from noisy or incomplete observation. Lellmann et al. [30] utilized the Kantorovich–Rubinstein discrepancy term together with a total variation (TV) term in the context of image denoising. They called their method *Kantorovich–Rubinstein-TV (KR-TV)* denoising. Note that the KR metric is closely related to the 1-Wasserstein metric (for 1-D signals they are equivalent). The KR term in their proposed functional provides a fidelity term for denoising, and the TV term enforces a piecewise constant reconstruction.

Transport-based morphometry

Given their suitability for comparing mass distributions, transport-based approaches for performing pattern recognition of morphometry encoded in image intensity values have also lately emerged. Recently described approaches for transport-based morphometry (TBM) [4], [27], [50] work by computing transport maps or plans between a set of images and a reference or template image. The transport plans/maps are then utilized as an invertible feature/transform onto which pattern recognition algorithms such as PCA or LDA can be applied. In effect, it utilizes the LOT framework described in the “The Linear Optimal Transportation Framework” section. These techniques have recently been employed to decode differences in cell and nuclear morphology for drug screening [4], cancer detection histopathology [39], and cytology images, as well as applications such as the analysis of galaxy morphologies [27].

Deformation-based methods have long been used in analyzing biomedical images. TBM, however, is different from

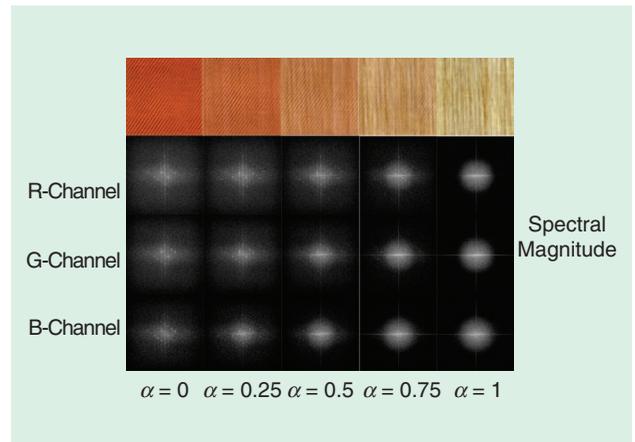


FIGURE 8. An example of texture mixing via optimal transport using the method presented in Ferradans et al. [18].

those deformation-based methods in that it has numerically exact, uniquely defined solutions for the transport plans or maps used; i.e., images can be matched with little perceptible error. The same is not true in methods that rely on registration via the computation of deformations, given the significant topology differences commonly found in medical images. Moreover, TBM allows for comparison of the entire intensity information present in the images (shapes and textures), while deformation-based methods are usually employed to deal with shape differences. Figure 9 shows a schematic of the TBM steps applied to a cell nuclei data set. It can be seen that TBM is capable of modeling the variation in the data set. In addition, it enables one to visualize the classifier, which discriminates between image classes (in this case malignant versus benign).

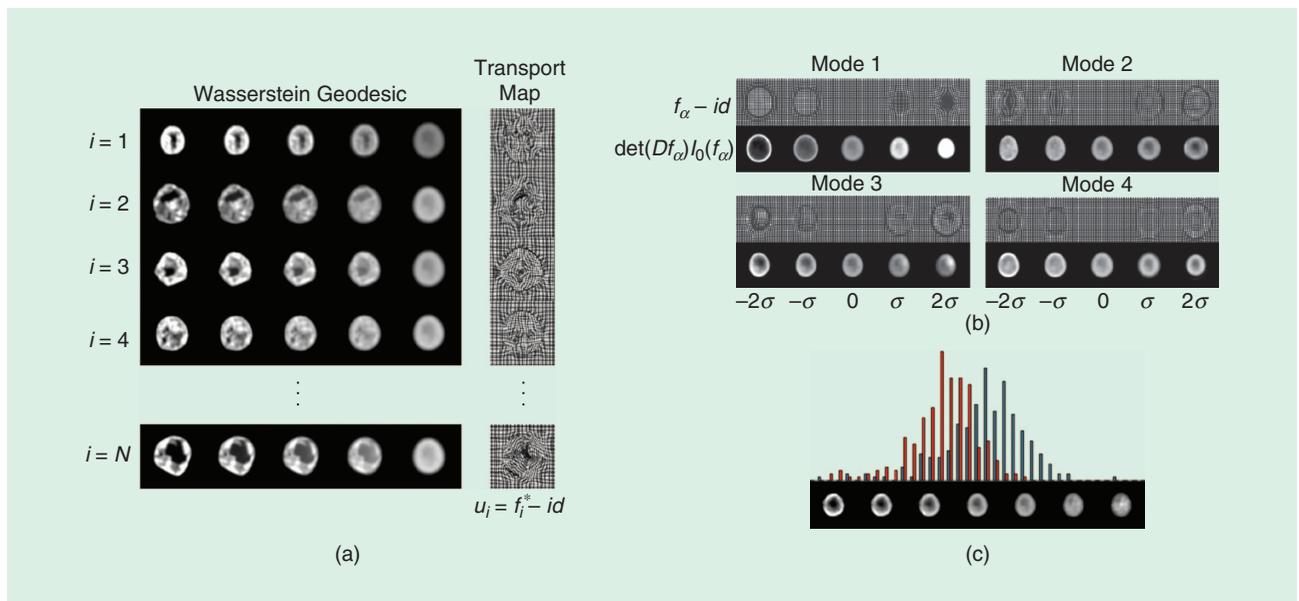


FIGURE 9. The schematic of the TBM framework. (a) The optimal transport maps between input images I_1, \dots, I_N and a template image I_0 are calculated. (b) and (c) Next, linear statistical modeling such as PCA, LDA, and canonical correlation analysis is performed on the optimal transport maps. The resulting transport maps obtained from the statistical modeling step are then applied to the template image to visualize the results of the analysis in the image space.

Superresolution

Superresolution is the process of reconstructing a high-resolution image from one or several corresponding low-resolution images. Superresolution algorithms can be broadly categorized into two major classes, multiframe superresolution and single-frame superresolution, based on the number of low-resolution images they require to reconstruct the corresponding high-resolution image. The TBM approach was used for single-frame superresolution in [26] to reconstruct high-resolution faces from very low-resolution-input face images. The authors utilized the TBM in combination with subspace learning techniques to learn a nonlinear model for the high-resolution face images in the training set.

In short, the method consists of a training and a testing phase. In the training phase, it uses high-resolution face images and morphs them to a template high-resolution face through optimal transport maps. Next, it learns a subspace

for the calculated optimal transport maps. A transport map in this subspace can then be applied to the template image to synthesize a high-resolution face image. In the testing phase, the goal is to reconstruct a high-resolution image from the low-resolution input image. The method searches for a synthetic high-resolution face image (generated from the transport subspace) that provides a corresponding low-resolution image, which is similar to the input low-resolution image. Figure 10 shows the steps used in this method and demonstrates reconstruction results.

Machine learning and statistics

The optimal transport framework has recently attracted ample attention from the machine-learning and statistics communities [12], [19], [25], [28], [36]. Some applications of the optimal transport in these arenas include various transport-based learning methods [19], [28], [36], [48], domain adaptation, Bayesian

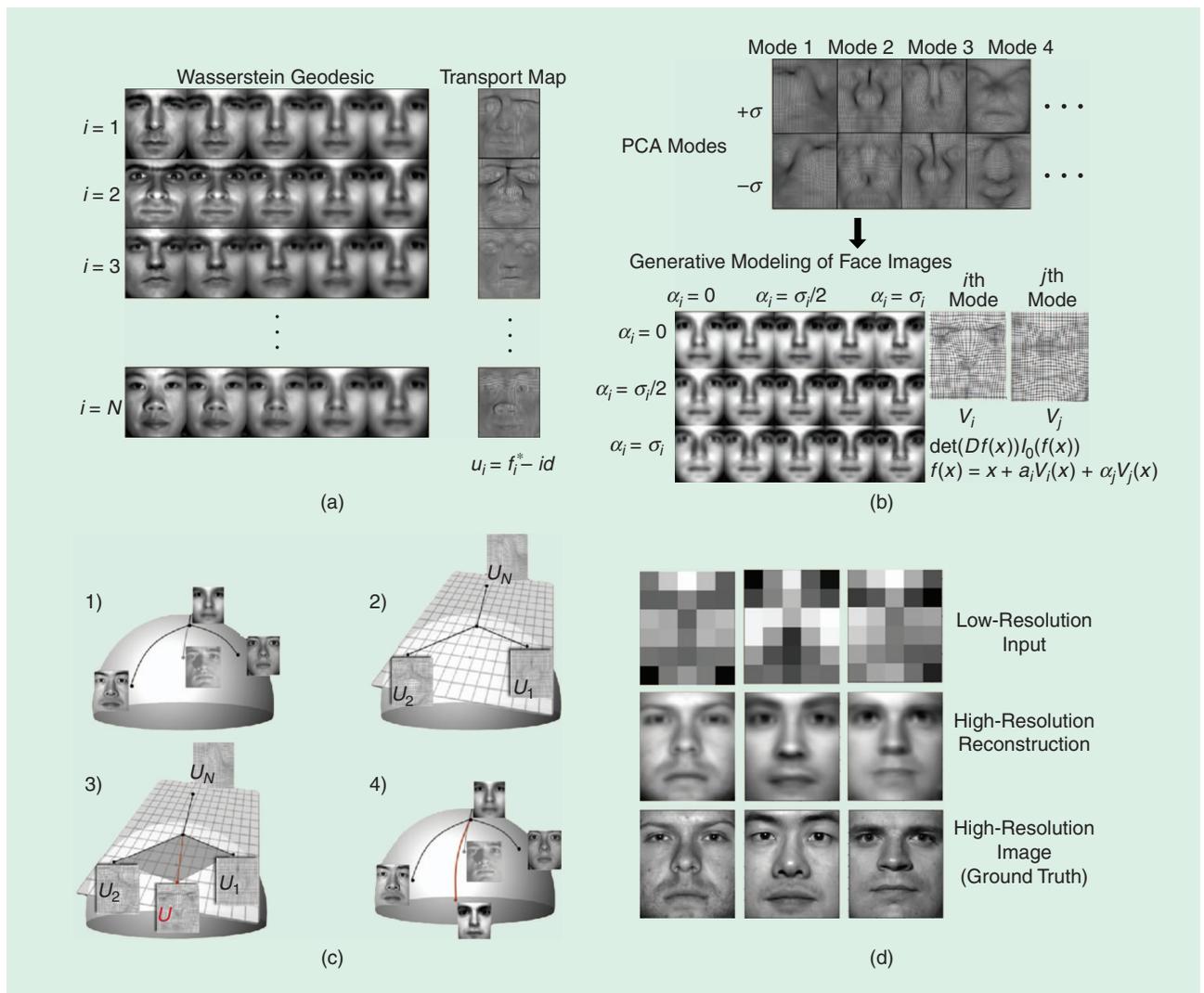


FIGURE 10. (a) In the training phase, optimal transport maps that morph the template image to high-resolution training face images are calculated. (b) Statistical modeling of transport maps. PCA is used to learn a linear subspace for transport maps for which a linear combination of obtained eigenmaps can be applied to the template image to obtain synthetic face images. (c) A geometric interpretation of the problem and (d) reconstruction results in transport-based single-frame superresolution. (Face portraits courtesy of the public Extended Yale Face Database B.)

inference [12], [13] and hypothesis testing [15], [42] among others. Here, we provide a brief overview of the recent developments of transport-based methods in machine learning and statistics.

Learning

Transport-based distances have recently been used in several works as a loss function for regression, classification, and other techniques. Montavon, Müller, and Cuturi [36], for instance, utilized the dual formulation of the entropy-regularized Wasserstein distance to train restricted Boltzmann machines (RBMs). Boltzmann machines are probabilistic graphical models (Markov random fields) that can be categorized as stochastic neural networks and are capable of extracting hierarchical features at multiple scales. RBMs are bipartite graphs that are special cases of Boltzmann machines, which define parameterized probability distributions over a set of d -binary input variables (observations) whose states are represented by h binary output variables (hidden variables). The parameters of RBMs are often learned through information theoretic divergences such as KL divergence. Montavon et al. [36] proposed an alternative approach through a scalable entropy-regularized Wasserstein distance estimator for RBMs and showed the practical advantages of this distance over the commonly used information divergence-based loss functions.

In another approach, Frogner et al. [19] used the entropy-regularized Wasserstein loss for multilabel classification. They proposed a relaxation of the transport problem to deal with unnormalized measures by replacing the equality constraints in (6) with soft penalties with respect to KL divergence. In addition, Frogner et al. [19] provided statistical bounds on the expected semantic distance between the prediction and the ground truth. In yet another approach, Kolouri et al. [28] utilized the sliced-Wasserstein metric and provided a family of positive definite kernels, denoted sliced-Wasserstein kernels, and showed the advantages of learning with such kernels. The sliced-Wasserstein kernels were shown to be effective in various machine-learning tasks, including classification, clustering, and regression.

Solomon et al. [48] considered the problem of graph-based semisupervised learning, in which graph nodes are partially labeled and the task is to propagate the labels throughout the nodes. Specifically, they considered a problem in which the labels are histograms. This problem arises, for example, in traffic density prediction, in which the traffic density is observed for a few stop lights over 24 h in a city and the city is interested in predicting the traffic density at the unobserved stop lights. They pose the problem as an optimization of a Dirichlet energy for distribution-valued maps based on the 2-Wasserstein distance and present a Wasserstein propagation scheme for semisupervised distribution propagation along graphs.

More recently, Arjovsky et al. [3] compared various distances, i.e., TV, KL divergence, Jensen–Shannon divergence, and the Wasserstein distance in training generative adversarial networks (GANs). They demonstrated (theoretically and numerically) that the Wasserstein distance leads to a superior performance compared to the later dissimilarity measures.

They specifically showed that their proposed Wasserstein GAN does not suffer from common issues in such networks, including instability and mode collapse.

Domain adaptation

Domain adaptation is one of the fundamental problems in machine learning that has gained proper attention from the machine-learning research community in the past decade. Domain adaptation is the task of transferring knowledge from classifiers trained on available labeled data to unlabeled test domains with data distributions that differ from that of the training data. The optimal transport framework was recently presented as a potential major player in domain adaptation problems [12], [13]. Courty et al. [12], for instance, assumed that there exists a nonrigid transformation between the source and target distributions, and they find this transformation using an entropy-regularized optimal transport problem. They also proposed a label-aware version of the problem in which the transport plan is regularized so a given target point (testing exemplar) is associated only with source points (training exemplars) belonging to the same class. Courty et al. [12] showed that domain adaptation via regularized optimal transport outperforms the state-of-the-art results in several challenging domain adaptation problems.

Bayesian inference

Another interesting and emerging application of the optimal transport problem is in Bayesian inference [17]. In Bayesian inference, one critical step is the evaluation of expectations with respect to a posterior probability function, which leads to complex multidimensional integrals. These integrals are commonly solved through the Monte Carlo numerical integration, which requires independent sampling from the posterior distribution. In practice, sampling from a general posterior distribution might be difficult, so, therefore, the sampling is performed via a Markov chain that converges to the posterior probability after a certain number of steps. This leads to the celebrated Markov chain Monte Carlo (MCMC) method. The downside of the MCMC method is that the samples are not independent, and, hence, the convergence of the empirical expectation is slow. El Moselhy and Marzouk [17] proposed a transport-based method that evades the need for Markov-chain simulation by allowing direct sampling from the posterior distribution. The core idea in their work is to find a transport map (via a regularized Monge formulation) that pushes forward the prior measure to the posterior measure. Then, sampling the prior distribution and applying the transport map to the samples will lead to a sampling scheme from the posterior distribution. Figure 11 shows the basic idea behind these methods.

Hypothesis testing

The Wasserstein distance is used for goodness-of-fit testing in [15] and for two-sample testing in [42]. Ramdas et al. [42] presented connections between the entropy-regularized Wasserstein distance, multivariate Energy distance, and the kernel maximum mean discrepancy and provided a “distribution-free” univariate Wasserstein test statistic. These and other

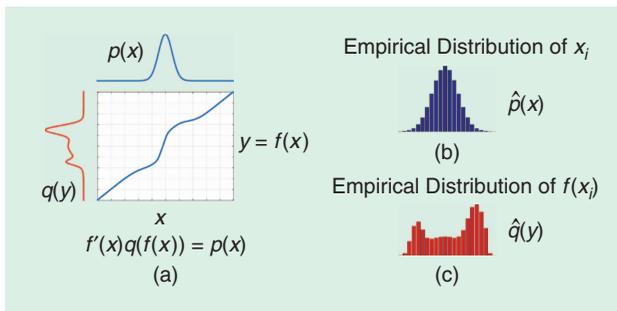


FIGURE 11. (a) The prior distribution p , the posterior distribution q , and the corresponding transport map f that pushes p into q . One million samples, x_i , were generated from distribution p . (b) The empirical distribution of these samples denoted as \hat{p} and (c) the empirical distribution of transformed samples, $y_i = f(x_i)$, denoted as \hat{q} .

applications of transport-related concepts show the promise of the mathematical modeling technique in the design of statistical data-analysis methods to tackle modern learning problems. Finally, note that, in the interest of brevity, a number of other important applications of transport-related techniques were not discussed above but are certainly interesting in their own right. For a more detailed discussion and more references please refer to [24].

Summary and conclusions

Transport-related methods and applications have come a long way. Although earlier applications focused primarily in civil engineering and economics problems, they have recently begun to be employed in a wide variety of problems related to signal and image analysis and pattern recognition. In this article, seven main areas of application were reviewed: image retrieval, registration and morphing, color transfer and texture analysis, image restoration, TBM, image superresolution, and machine learning and statistics. Transport and related techniques have gained increased interest in recent years. Overall, researchers have found that the application of transport-related concepts can be helpful in solving problems in diverse applications. Given recent trends, it seems safe to expect that the number of application areas will continue to grow.

In its most general form, the transport-related techniques reviewed in this article can be thought as mathematical models for signals and images and in general data distributions. Transport-related metrics involve calculating differences not only of pixel or distribution intensities but also where they are located in the corresponding coordinate space (a pixel coordinate in an image or a particular axis in some arbitrary feature space). As such, the geometry (e.g., geodesics) induced by such metrics can give rise to dramatically different algorithms and data interpretation results. The interesting performance improvements recently obtained could motivate the search for a more rigorous mathematical understanding of transport-related metrics and applications.

The emergence of numerically precise and efficient ways of computing transport-related metrics and geodesics, as presented in the “Numerical Methods” section, also serves as an enabling mechanism. Coupled with the fact that several

mathematical properties of transport-based metrics have been extensively studied, we believe that the foundation is set for their increased use as tools or building blocks based on which complex computational systems can be built. The confluence of these emerging ideas may spur a significant amount of innovation in a world where sensor and other data are becoming abundant and computational intelligence to analyze these is in high demand. We believe transport-based models will become an important component of the ever-expanding tool set available to modern signal-processing and data-science experts.

Acknowledgments

We gratefully acknowledge funding from the National Science Foundation (NSF) (CCF 1421502) and the National Institutes of Health (GM090033, CA188938) in contributing to a portion of this work. Dejan Slepčev also acknowledges funding by the NSF (DMS DMS-1516677).

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