Rectified Flow: A Marginal Preserving Approach to Optimal Transport

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Abstract

We present a flow-based approach to the optimal transport (OT) problem between two continuous distributions π_0, π_1 on $\mathbb{R}^d$, of minimizing a transport cost $\mathbb{E}[c(X_1 - X_0)]$ in the set of couplings (X_0, X_1) whose marginal distributions on X_0, X_1 equals π_0, π_1, respectively, where c is a cost function. Our method iteratively constructs a sequence of neural ordinary differentiable equations (ODE), each learned by solving a simple unconstrained regression problem, which monotonically reduce the transport cost while automatically preserving the marginal constraints. This yields a monotonic *interior* approach that traverses inside the set of valid couplings to decrease the transport cost, which distinguishes itself from most existing approaches that enforce the coupling constraints from the outside. The main idea of the method draws from *rectified flow* [LGL22], a recent approach that simultaneously decreases the whole family of transport costs induced by convex functions c (and is hence *multi-objective* in nature), but is not tailored to minimize a specific transport cost. Our method is a *single-object* variant of rectified flow that guarantees to solve the OT problem for a fixed, user-specified convex cost function c.

1 Introduction

The Monge–Kantorovich (MK) optimal transport (OT) problem concerns finding an optimal coupling between two distributions π_0, π_1:

$$\inf_{(X_0, X_1)} \mathbb{E}[c(X_1 - X_0)], \quad s.t. \quad \mathrm{Law}(X_0) = \pi_0, \ \mathrm{Law}(X_1) = \pi_1, \tag{1}$$

where we seek to find (the law of) an optimal coupling (X_0, X_1) of π_0 and π_1, for which marginal laws of X_0, X_1 equal π_0, π_1, respectively, to minimize $\mathbb{E}[c(X_1 - X_0)]$, called the c-transport cost, for a cost function c. Theories, algorithms, and applications of optimal transport have attracted a vast literature; see, for example, the monographs of [Vil21, Vil09, ABS21, San15, PC+19] for overviews. Notably, OT has been growing into a popular and powerful technique in machine learning, for key tasks such as learning generative models, transfer learning, and approximate inference [e.g., PC+19, ACB17, SRGB14, EMM12, CFT14, MMPS16].

The OT problem should be treated differently depending on whether π_0, π_1 are discrete or continuous measures. In this work, we focus on the continuous case when π_0, π_1 are high dimensional absolutely continuous measures on $\mathbb{R}^d$ that are observed through empirical observations, a setting called data-driven OT in [TT16]. A well known result in OT [e.g., Vil09] shows that, if π_0 is continuous, the optimization in

(1) can be restricted to the set of deterministic couplings satisfying $X_1 = T(X_0)$ for some continuous transport mapping $T\colon \mathbb{R}^d \to \mathbb{R}^d$, which is often approximated in practice with deep neural networks [e.g., MTOL20, KLG+21, KSB22, HCTC20].

However, continuous OT remains highly challenging computationally. One major difficulty is to handle the coupling constraints of $\mathrm{Law}(X_0) = \pi_0$ and $\mathrm{Law}(X_1) = \pi_1$, which are infinite dimensional when π_0 and π_1 are continuous. As a result, (1) can not be solved as a "clean" unconstrained optimization problem. There are essentially two types of approaches to solving (1) in the literature. One uses Lagrange duality to turn (1) into a certain minimax game, and the other one approximates the constraint with an integral (often entropic-like) penalty function. However, the minimax approaches suffer from convergence and instability issues and are difficult to solve in practice, while the regularization approach can not effectively enforce the infinite-dimensional coupling constraints.

This work We present a different approach to continuous OT that re-frames (1) into a sequence of simple unconstrained nonlinear least squares optimization problems, which monotonically reduce the transport cost of a coupling while automatically preserving the marginal constraints. Different from the minimax and regularization approaches that enforce the constraints from outside, our method is an *interior* approach which starts from a valid coupling (typically the naive independent coupling), and traverses inside the constraint set to decrease the transport cost. Such an interior approach is non-trivial and has not been realized before, because there exists no obvious unconstrained parameterization of the set of couplings of π_0 and π_1.

Our method is made possible by leveraging *rectified flow* [LGL22], a recent approach to constructing (non-optimal) transport maps for generative modeling and domain transfer. What makes rectified flow special is that it provides a simple procedure that turns a given coupling into a new one that obeys the same marginal laws, while yielding no worse transport cost w.r.t. *all* convex functions c simultaneously. Despite this attractive property, as pointed out in [LGL22], rectified flow can not be used to optimize any fixed cost c, as it is essentially a special *multi-objective* optimization procedure that targets no specific cost. Our method is a variant of rectified flow that targets a user-specified cost function c and hence yields a new approach to the OT problem (1).

Rectified flow We provide a high-level overview of the rectified flow of [LGL22] and the main results of this work. For a given coupling (X_0, X_1) of π_0 and π_1, the *rectified flow* induced by (X_0, X_1) is the time-differentiable process $\boldsymbol{Z} = \{Z_t\colon t \in [0,1]\}$ over an artificial notion of time $t \in [0,1]$, that solves the following ordinary differential equation (ODE):

$$\mathrm{d}Z_t = v_t^X(Z_t)\mathrm{d}t, \quad t \in [0,1], \quad \text{starting from} \quad Z_0 = X_0, \tag{2}$$

where $v^X\colon \mathbb{R}^d \times [0,1] \to \mathbb{R}^d$ is a time-dependent velocity field defined as the solution of

$$\inf_v \int_0^1 \mathbb{E}\left[\|X_1 - X_0 - v(X_t, t)\|^2\right]\mathrm{d}t, \qquad X_t = tX_1 + (1-t)X_0, \tag{3}$$

and X_t is the linear interpolation between X_0 and X_1. Eq (3) is a least squares regression problem of predicting the line direction of $(X_1 - X_0)$ from every space-time point (X_t, t) on the linear interpolation path, yielding a solution of

$$v_t^X(z) = \mathbb{E}\left[X_1 - X_0 \mid X_t = z\right],$$

which is the average of direction $(X_1 - X_0)$ for all lines that pass point $X_t = z$ at time t. The (conditional) expectations $\mathbb{E}[\cdot]$ above are w.r.t. the randomness of (X_0, X_1). We assume that the solution of (2) exists

and is unique, and hence $v_t^X(z)$ is assumed to exist at least on the trajectories of the ODE. The start-end pair (Z_0, Z_1) induced by $\boldsymbol{Z}$ is called the *rectified coupling* of (X_0, X_1), and we denote it by $(Z_0, Z_1) = \texttt{Rectify}((X_0, X_1))$.

In practice, the expectation $\mathbb{E}[\cdot]$ is approximated by empirical observations of (X_0, X_1), and v is approximated by a parametric family, such as deep neural networks. In this case, the optimization in Eq (3) can be solved conveniently with off-the-shelf stochastic optimizers such as stochastic gradient descent (SGD), without resorting to minimax algorithms or expensive inner loops. This makes rectified flow attractive for deep learning applications as these considered in [LGL22].

The importance of $(Z_0, Z_1) = \texttt{Rectify}((X_0, X_1))$ is justified by two key properties:

1) (Z_0, Z_1) *shares the same marginal laws as* (X_0, X_1) *and is hence a valid coupling of* π_0 *and* π_1;

2) (Z_0, Z_1) *yields no larger convex transport costs than* (X_0, X_1), *that is,* $\mathbb{E}[c(Z_1 - Z_0)] \leq \mathbb{E}[c(X_1 - X_0)]$, *for* every *convex function* $c \colon \mathbb{R}^d \to \mathbb{R}$.

Hence, it is natural to recursively apply the $\texttt{Rectify}$ mapping, that is, $(Z_0^{k+1}, Z_1^{k+1}) = \texttt{Rectify}((Z_0^k, Z_1^k))$ starting from $(Z_0^0, Z_1^0) = (X_0, X_1)$, yielding a sequence of couplings that is monotonically non-increasing in terms of all convex transport costs. The initialization can be taken to be the independent coupling $(Z_0^0, Z_1^0) \sim \pi_0 \times \pi_1$, or any other couplings that can be constructed from marginal (unpaired) observations of π_0 and π_1. In practice, each step of $\texttt{Rectify}$ is empirically approximated by first drawing samples of (Z_0^k, Z_1^k) from the ODE with drift v^k, and then constructing the next flow v^{k+1} from the optimization in (3). Although this process accumulates errors, it was shown that one or two iterations are sufficient for practical applications [LGL22].

Note that the $\texttt{Rectify}$ procedure is "cost-agnostic" in that it does not dependent on any specific cost c. Although the recursive $\texttt{Rectify}$ update is monotonically non-increasing on the transport cost for all convex c, it does not necessarily converge to the optimal coupling for any pre-specified c, as the update would stop whenever two cost functions are conflicting with each other. In [LGL22], a coupling (X_0, X_1) is called *straight* if it is a fixed point of $\texttt{Rectify}$, that is, $(X_0, X_1) = \texttt{Rectify}((X_0, X_1))$. It was shown that rectifiable couplings that are optimal w.r.t. a convex c must be straight, but the opposite is not true in general. One exception is the one dimension case ($d = 1$), for which all convex functions c (whose c-optimal coupling exists) share a common optimal coupling that is also straight. But this does not hold when $d \geq 2$.

c-**Rectified flow**   In this work, we modify the $\texttt{Rectify}$ procedure so that it can be used to solve (1) given a user-specified cost function c. We show that this can be done easily by properly restricting the optimization domain of v and modifying the loss function in (3). The case of quadratic loss $c(x) = \frac{1}{2}\|x\|^2$ is particularly simple, for which we simply need to restrict the v to be a gradient field $v_t = \nabla f_t$ in the optimization of (3). For more general convex c, we need to restrict v to have a form of $v_t(x) = \nabla c^*(\nabla f_t(x))$, with f minimizing the following loss function:

$$\inf_f \int_0^1 \mathbb{E}\left[c^*(\nabla f(X_t)) - (X_1 - X_0)^\top \nabla f(X_t) + c(X_1 - X_0)\right] \mathrm{d}t, \tag{4}$$

where c^* denotes the conjugate function of c. Obviously when $c(x) = \frac{1}{2}\|x\|^2$, (4) reduces to (3) with $v = \nabla f$. The loss function in (4) is closely related to *Bregman divergence* [e.g., BMD$^+$05] and the so-called *matching loss* [e.g., AHW95]. We call $\boldsymbol{Z} = \{Z_t \colon t \in [0,1]\}$ that follows $\mathrm{d}Z_t = \nabla c^*(\nabla f_t(Z_t))\mathrm{d}t$

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with $Z_0 = X_0$ and f solving (4) the c-rectified flow of (X_0, X_1), and the corresponding (Z_0, Z_1) the c-rectified coupling of (X_0, X_1), denoted as $(Z_0, Z_1) = c\text{-Rectify}((X_0, X_1))$.

Similar to the original rectified coupling, the c-rectified coupling (Z_0, Z_1) also share the same marginal laws as (X_0, X_1) and hence is a coupling of π_0 and π_1. In addition, (Z_0, Z_1) yields no larger transport cost than (X_0, X_1) w.r.t. c, that is, $\mathbb{E}[c(Z_1 - Z_0)] \leq \mathbb{E}[c(X_1 - X_0)]$. But this only holds for the specific c that is used to define the flow, rather than all convex functions like Rectify.

More importantly, recursively performing c-Rectify allows us to find c-optimal couplings that solve the OT problem (1). Under mild conditions, we have

$$(X_0, X_1) = c\text{-Rectify}((X_0, X_1)) \quad \Longleftrightarrow \quad (X_0, X_1) \text{ is } c\text{-optimal in (1)} \quad \Longleftrightarrow \quad \ell_{X,c}^* = 0,$$

where $\ell_{X,c}^*$ denotes the minimum value of the loss function in (4), which provides a criterion of c-optimality of a given coupling without solving the OT problem. Moreover, when following the recursive update $(Z_0^{k+1}, Z_1^{k+1}) = c\text{-Rectify}((Z_0^k, Z_1^k))$, the $\ell_{Z^k,c}^*$ is guaranteed to decay to zero with $\min_{k \leq K} \ell_{Z^k,c}^* = O(1/K)$.

Notation   Let $C^1(\mathbb{R}^d)$ be the set of continuously differentiable functions $f \colon \mathbb{R}^d \to \mathbb{R}$, and $C_c^1(\mathbb{R}^d)$ the functions in $C^1(\mathbb{R}^d)$ whose support is compact. For a time-dependent velocity field $v \colon \mathbb{R}^d \times [0, 1] \to \mathbb{R}$, we write $v_t(\cdot) = v(x, t)$ and use $\dot{v}_t(x) := \partial v(x, t)$ and $\nabla v_t(x) := \partial_x v(x, t)$ to denote the partial derivative w.r.t. time t and variable x, respectively. We denote by $C^{2,1}(\mathbb{R}^d \times [0, 1])$ the set of functions $f \colon \mathbb{R}^d \times [0, 1] \to \mathbb{R}$ that are second-order continuously differentiable w.r.t. x and first-order continuously differentiable w.r.t. t. In this work, an ordinary differential equation (ODE) $\mathrm{d}z_t = v_t(z_t)\mathrm{d}t$ should be interpolated as an integral equation $z_t = z_0 + \int_0^t v_t(z_t)\mathrm{d}t$. For $x \in \mathbb{R}^d$, $\|x\|$ denotes the Euclidean norm. We always write c^* as the convex conjugate of $c \colon \mathbb{R}^d \to \mathbb{R}$, that is, $c^*(x) = \sup_{y \in \mathbb{R}^d} \{x^\top y - c(y)\}$.

Random variables are capitalized (e.g., X, Y, Z) to distinguish them with deterministic values (e.g, x, y, z). Recall that an $\mathbb{R}^d$-valued random variable $X = X(\omega)$ is a measurable function $X \colon \Omega \to \mathbb{R}^d$, where Ω is an underlying sample space equipped with a σ-algebra $\mathcal{F}$ and a probability measure $\mathbb{P}$. The triplet $(\Omega, \mathcal{F}, \mathbb{P})$ form the underlying probability space, which is omitted in writing in the most places. We use $\mathrm{Law}(X)$ to denote the probability law of X, which is the probability measure $\mathbb{L}$ that satisfies $\mathbb{L}(B) = \mathbb{P}(\{\omega \colon X(\omega) \in B\})$ for all measurable sets on $\mathbb{R}^d$. For a functional $F(X)$ of a random variable X, the optimization problem $\min_X F(X)$ technically means to find a measurable function $X(\omega)$ to minimize F, even though we omit the underlying sample space Ω. When $F(X)$ depends on X only through $\mathrm{Law}(X)$, the optimization problem is equivalent to finding the optimal $\mathrm{Law}(X)$.

Outline   The rest of the work is organized as follows. Section 2 introduces the background of optimal transport. Section 3 reviews rectified flow of [LGL22] from an optimization-based view. Section 4 characterizes the if and only if condition for two differentiable stochastic processes to have equal marginal laws. Section 5 introduces the main c-rectified flow method and establishes its theoretical properties.

2   Background of Optimal Transport

This section introduces the background of optimal transport (OT), including both the static and dynamic formulations. Of special importance is the dynamic formulation, which is closely related to the rectified

flow approach. The readers can find systematic introductions to OT in a collection of excellent textbooks [Vil21, FG21, ABS21, PC$^+$19, OPV14, San15, Vil09].

Static formulations   The optimal transport problem was first formulated by Gaspard Monge in 1781 when he studied the problem of how to redistribute mass, e.g., a pile of soil, with minimal effort. Monge's problem can be formulated as

$$\inf_{T} \mathbb{E}\left[c(T(X_0) - X_0)\right] \quad s.t. \quad \mathrm{Law}(T(X_0)) = \pi_1, \quad \mathrm{Law}(X_0) = \pi_0, \tag{5}$$

where we minimize the c-transport cost in the set of deterministic couplings (X_0, X_1) that satisfy $X_1 = T(X_0)$ for a transport mapping $T \colon \mathbb{R}^d \to \mathbb{R}^d$. The Monge–Kantorovich (MK) problem in (1) is the relaxation of (5) to the set of all (deterministic and stochastic) couplings of π_0 and π_1. The two problems are equivalent when the optimum of (1) is achieved by a deterministic coupling, which is guaranteed if π_0 is an absolutely continuous measure on $\mathbb{R}^d$.

A key feature of the MK problem is that it is a linear programming w.r.t. the law of the coupling (X_0, X_1), and yields a dual problem of form:

$$\sup_{\mu,\nu} \pi_1(\mu) - \pi_0(\nu) \ \ s.t. \ \ \mu(x_1) - \nu(x_0) \leq c(x_1 - x_0), \quad \forall(x_0, x_1), \tag{6}$$

where we write $\pi_1(\mu) := \int \mu(x) \mathrm{d}\pi_1(x)$, and μ, ν are optimized in all functions from $\mathbb{R}^d$ to $\mathbb{R}$. For any coupling (X_0, X_1) of π_0 and π_1, and (μ, ν) satisfying the constraint in (6), it is easy to see that

$$\mathbb{E}[c(X_1 - X_0)] \geq \mathbb{E}[\mu(X_1) - \nu(X_0)] = \pi_1(\mu) - \pi_0(\nu). \tag{7}$$

As the left side of (7) only depends on (X_0, X_1) and the right side only on (μ, ν), one can show that (X_0, X_1) is c-optimal and (μ, ν) solves (6) iff $\mu(X_0) + \nu(X_1) = c(X_1 - X_0)$ holds with probability one, which provides a basic optimality criterion. Many existing OT algorithms are developed by exploiting the primal dual relation of (1) and (6) (see e.g., [KSB22]), but have the drawback of yielding minimax problems that are challenging to solve in practice.

If c is strictly convex, the optimal transport map of (5) is unique (almost surely) and yields a form of

$$T(x) = x + \nabla c^*(\nabla \nu(x)),$$

where c^* is the convex conjugate function of c, and ν is an optimal solution of (6), which is c-convex in that $\nu(x) = \sup_y \{-c(y - x) + \mu(y)\}$ with μ the associated solution. In the canonical case of quadratic cost $c(x) = \frac{1}{2}\|x\|^2$, we can write $T(x) = \nabla \phi(x)$, where $\phi(x) := \frac{1}{2}\|x\|^2 + \nu(x)$ is a convex function.

Dynamic formulations   Both the MK and Monge problems can be equivalently framed in dynamic ways as finding continuous-time processes that transfer π_0 to π_1. Let $\{x_t \colon t \in [0, 1]\}$ be a smooth path connecting x_0 and x_1, whose time derivative is denoted as $\dot{x}_t$. For convex c, by Jensen's inequality, we can represent the cost $c(x_1 - x_0)$ in an integral form:

$$c(x_1 - x_0) = c\left(\int_0^1 \dot{x}_t \mathrm{d}t\right) = \inf_x \int_0^1 c(\dot{x}_t) \mathrm{d}t,$$

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where the infimum is attained when x_t is the linear interpolation (geodesic) path: $x_t = tx_1 + (1-t)x_0$. Hence, the MK optimal transport problem (1) is equivalent to

$$\inf_{\boldsymbol{X}} \mathbb{E}\left[\int_0^1 c(\dot{X}_t)\mathrm{d}t\right] \quad s.t. \quad \mathrm{Law}(X_0) = \pi_0, \ \mathrm{Law}(X_1) = \pi_1, \tag{8}$$

where we optimize in the set of time-differentiable stochastic processes $\boldsymbol{X} = \{X_t \colon t \in [0,1]\}$. The optimum of (8) is attained by $X_t = tX_1 + (1-t)X_0$ when (X_0, X_1) is a c-optimal coupling of (1), which is known as the *displacement interpolation* [McC97]. We call the objective function in (8) the path-wise c-transport cost.

The Monge problem can also be framed in a dynamic way. Assume the transport map T can be induced by an ODE model $\mathrm{d}X_t = v_t(X_t)\mathrm{d}t$ such that $X_1 = T(X_0)$. Then the Monge problem is equivalent to

$$\inf_{v,\boldsymbol{X}} \mathbb{E}\left[\int_0^1 c(v_t(X_t))\mathrm{d}t\right] \quad s.t. \quad \mathrm{d}X_t = v_t(X_t)\mathrm{d}t, \quad \mathrm{Law}(X_0) = \pi_0, \quad \mathrm{Law}(X_1) = \pi_1, \tag{9}$$

which is equivalent to restricting $\boldsymbol{X}$ in (8) to the set of processes that can be induced by ODEs.

Assume that X_t following $\mathrm{d}X_t = v_t(X_t)\mathrm{d}t$ yields a density function ϱ_t. Then it is well known that ϱ_t satisfies the continuity equation:

$$\dot{\varrho}_t + \nabla \cdot (v_t \varrho_t) = 0.$$

Hence, we can rewrite (9) into an optimization problem on (v, ϱ), yielding the celebrated *Benamou-Brenier formula* [BB00]:

$$\inf_{v,\varrho} \int_0^1 \int c(v_t(x))\varrho_t(x)\mathrm{d}x\mathrm{d}t \quad s.t. \quad \dot{\varrho}_t + \nabla \cdot (v_t\varrho_t) = 0, \quad \rho_0 = \mathrm{d}\pi_0/\mathrm{d}x, \quad \rho_1 = \mathrm{d}\pi_1/\mathrm{d}x, \tag{10}$$

where $\mathrm{d}\pi_i/\mathrm{d}x$ denotes the density function of π_i. The key idea of (9) and (10) is to restrict the optimization of (8) to the set of deterministic processed induced by ODEs, which significantly reduces the search space. Intuitively, Jensen's inequality $\mathbb{E}[c(Z)] \geq c(\mathbb{E}[Z])$ shows that we should be able to reduce the expected cost of a stochastic process by "marginalizing" out the randomness. In fact, we will show that, for a differentiable stochastic process $\boldsymbol{X}$, its (c-)rectified flow yields no larger path-wise c-transport cost in (8) than $\boldsymbol{X}$ (see Lemma 3.3 and Theorem 5.3).

However, all the dynamic formulations above are still highly challenging to solve in practice. We will show that c-rectified flow can be viewed as a special coordinate descent like approach to solving (8) (Section 5.4).

3   Rectified Flow: An Optimization-Based View

We introduce rectified flow of [LGL22] from an optimization-based perspective: we show that rectified flow can be viewed as the solution of a special constrained dynamic optimization problem, which allows us to gain more understanding of rectified flow and motivates the development of c-rectified flow.

Following [LGL22], for a time-differentiable stochastic process $\boldsymbol{X} = \{X_t \colon t \in [0,1]\}$, its expected velocity field $v^{\boldsymbol{X}}$ is defined as

$$v_t^{\boldsymbol{X}}(z) = \mathbb{E}[\dot{X}_t \mid X_t = z]. \tag{11}$$

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where $\dot{X}_t$ denotes the time derivative of X_t. Obviously, $v^{\boldsymbol{X}}$ is the solution of

$$\inf_v \left\{ L_{\boldsymbol{X}}(v) := \int_0^1 \mathbb{E}\left[\left\| \dot{X}_t - v_t(X_t) \right\|^2 \right] \mathrm{d}t \right\}, \tag{12}$$

where the optimization is on the set of all measurable velocity fields $v \colon \mathbb{R}^d \to \mathbb{R}^d$. The importance of $v^{\boldsymbol{X}}$ lies on the fact that it characterizes the time-evolution of the marginal laws $\rho_t := \mathrm{Law}(X_t)$ of $\boldsymbol{X}$, through the continuity equation in the distributional sense:

$$\partial_t \rho_t + \nabla \cdot (v_t^{\boldsymbol{X}} \rho_t) = 0, \quad \rho_0 = \mathrm{Law}(X_0), \quad t \in [0,1]. \tag{13}$$

Precisely, Equation (13) should be interpreted by its weak and integral form:

$$\rho_t(h) - \rho_0(h) - \int_0^t \rho_t(\nabla h^\top v_s^{\boldsymbol{X}}) \mathrm{d}s = 0, \quad \rho_0 = \mathrm{Law}(X_0), \quad \forall h \in C_c^1(\mathbb{R}^d), \quad t \in [0,1], \tag{14}$$

where $\rho_t(h) := \int h(x) \mathrm{d}\rho_t(x)$ and $C_c^1(\mathbb{R}^d)$ denotes the set of continuously differentiable functions on $\mathbb{R}^d$ with compact support. Hence, if the solution of Eq (13)-(14) is unique, then the marginal laws $\{\mathrm{Law}(X_t)\}_t$ of $\boldsymbol{X}$ are uniquely determined by $v^{\boldsymbol{X}}$ and the initial $\mathrm{Law}(X_0)$.

We define the rectified flow of $\boldsymbol{X}$, denoted by $\boldsymbol{Z} = \mathtt{Rectflow}(\boldsymbol{X})$, as the ODE driven by $v^{\boldsymbol{X}}$:

$$\mathrm{d}Z_t = v_t^{\boldsymbol{X}}(Z_t)\mathrm{d}t, \quad Z_0 = X_0, \quad t \in [0,1]. \tag{15}$$

Moreover, the rectified flow of a coupling (X_0, X_1) is defined as the rectified flow of $\boldsymbol{X}$ when $\boldsymbol{X}$ is the linear interpolation of (X_0, X_1).

Definition 3.1. *A stochastic process $\boldsymbol{X}$ is called rectifiable if $v^{\boldsymbol{X}}$ exists and is locally bounded, and Equation (15) has an unique solution.*

A coupling (X_0, X_1) is called rectifiable if its linear interpolation process $\boldsymbol{X}$, following $X_t = tX_1 + (1 - t)X_0$, is rectifiable. In this case, we call $\boldsymbol{Z} = \mathtt{Rectflow}(\boldsymbol{X})$ the rectified flow of (X_0, X_1), and write it (with an abuse of notation) as $\boldsymbol{Z} = \mathtt{Rectflow}((X_0, X_1))$. The corresponding (Z_0, Z_1) is called the rectified coupling of (X_0, X_1), denoted as $(Z_0, Z_1) = \mathtt{Rectify}((X_0, X_1))$.

By the definition in (15), we have $v^{\boldsymbol{Z}} = v^{\boldsymbol{X}}$, and hence the marginal laws $\mathrm{Law}(Z_t)$ of $\boldsymbol{Z}$ are governed by the same continuity equation (13)-(14), which is a well known fact. As shown in [Kur11], Equation (15) has an unique solution iff Equation (14) has an unique solution, which implies that $\boldsymbol{Z}$ and $\boldsymbol{X}$ share the same marginal laws. We also assumed that the solution of (12) is unique; if not, results in the paper hold for all solutions of (12).

Theorem 3.2 (Theorem 3.3 of [LGL22]). *Assume that $\boldsymbol{X}$ is rectifiable. We have*

$$\boldsymbol{Z} = \mathtt{Rectflow}(\boldsymbol{X}) \qquad \Rightarrow \qquad v^{\boldsymbol{X}} = v^{\boldsymbol{Z}} \qquad \Rightarrow \qquad \mathrm{Law}(X_t) = \mathrm{Law}(Z_t), \ \forall t \in [0,1].$$

Hence, rectified flow turns a rectifiable stochastic process into a flow while preserving the marginal laws.

A optimization view of rectified flow   We show that the rectified flow $\boldsymbol{Z}$ of $\boldsymbol{X}$ achieves the minimum of the path-wise c-transport cost in the set of time-differentiable stochastic processes whose expected velocity field equals $v^{\boldsymbol{X}}$. This explains that the property of non-increasing convex transport costs of rectified flow/coupling.

Lemma 3.3. *The rectified flow* $\boldsymbol{Z} = \texttt{Rectflow}(\boldsymbol{X}_t)$ *in* (15) *attains the minimum of*

$$\inf_{\boldsymbol{Y}} \left\{ F_c(\boldsymbol{Y}) := \int_0^1 \mathbb{E}\left[c(\dot{Y}_t)\right] \mathrm{d}t, \quad s.t. \quad v^{\boldsymbol{Y}} = v^{\boldsymbol{X}} \right\}, \tag{16}$$

which holds for any *convex functions* $c \colon \mathbb{R}^d \to \mathbb{R}$.

Proof. For any stochastic process $\boldsymbol{Y}$ with $v_t^{\boldsymbol{X}}(z) = v_t^{\boldsymbol{Y}}(z) = \mathbb{E}[\dot{Y}_t | Y_t = z]$, we have

$$
\begin{aligned}
F_c(\boldsymbol{Y}) &= \int_0^1 \mathbb{E}[c(\dot{Y}_t)]\mathrm{d}t \\
&\geq \int_0^1 \mathbb{E}[c(\mathbb{E}[\dot{Y}_t | Y_t])]\mathrm{d}t \qquad \text{//Jensen's inequality} \\
&= \int_0^1 \mathbb{E}[c(v^{\boldsymbol{Y}}(Y_t))]\mathrm{d}t \\
&= \int_0^1 \mathbb{E}[c(v^{\boldsymbol{X}}(X_t))]\mathrm{d}t \qquad \text{//}v^{\boldsymbol{X}} = v^{\boldsymbol{Y}}, \text{ and hence } \mathrm{Law}(X_t) = \mathrm{Law}(Y_t) \\
&= \int_0^1 \mathbb{E}[c(v^{\boldsymbol{X}}(Z_t))]\mathrm{d}t \qquad \text{//}\mathrm{Law}(X_t) = \mathrm{Law}(Z_t) \\
&= \int_0^1 \mathbb{E}[c(\dot{Z}_t)\mathrm{d}t = \boldsymbol{F}_c(\boldsymbol{Z}).
\end{aligned}
$$

$\square$

Lemma 3.3 suggests that the rectified flow decreases the path-wise c-transport cost: $F_c(\boldsymbol{Z}) \leq F_c(\boldsymbol{X})$, for all convex c. Note that $\mathbb{E}\left[c(Z_1 - Z_0)\right] \leq F_c(\boldsymbol{Z})$ by Jensen's inequality, and $\mathbb{E}\left[c(X_1 - X_0)\right] = F_c(\boldsymbol{X})$ if $\boldsymbol{X}$ is the linear interpolation of (X_0, X_1). Hence, in this case, we have

$$\mathbb{E}[c(Z_1 - Z_0)] \leq F_c(\boldsymbol{Z}) \leq F_c(\boldsymbol{X}) = \mathbb{E}[c(X_1 - X_0)],$$

which yields a proof of Theorem 3.2 of [LGL22] that the rectified coupling (Z_0, Z_1) yields no larger convex transport costs than (X_0, X_1).

A primal-dual relation   Let us generalize the least squares loss $L_{\boldsymbol{X}}(v)$ in (12) to a a Bregman divergence based loss:

$$\tilde{L}_{\boldsymbol{X},c}(v) := \int_0^1 \mathbb{E}\left[\mathsf{b}_c\Big(\dot{X}_t;\ v_t(X_t)\Big)\right] \mathrm{d}t, \qquad \mathsf{b}_c(x; y) = c(x) - c(y) - (x - y)^\top \nabla c(y),$$

where $\mathsf{b}_c(\cdot\,; \cdot)$ is the Bregman divergence w.r.t. c. The least squares loss $L_{\boldsymbol{X}}$ is recovered with $c(x) = \frac{1}{2}\|x\|^2$.

Rectified flow can be alternatively implemented by minimizing $\tilde{L}_{\boldsymbol{X},c}$ with a differentiable strictly convex c, as in this case the minimum of $\tilde{L}_{\boldsymbol{X},c}$ is also attended by $v^{\boldsymbol{X}}(z) = \mathbb{E}[\dot{X}_t|X_t = z]$. The c-rectified flow is obtained if we minimize $\tilde{L}_{\boldsymbol{X},c}$ with v restricted to be a form of $v = \nabla c^* \circ \nabla f_t$. See more in Section 5.

In the following, we show that the optimization in (16) can be viewed as the dual problem (11).

Theorem 3.4. *For any differentiable convex function c, and rectifiable process $\boldsymbol{X}$, we have*

$$\tilde{\ell}^*_{\boldsymbol{X},c} := \inf_v \tilde{L}_{\boldsymbol{X},c}(v) = \sup_{\boldsymbol{Y}} \left\{ F_c(\boldsymbol{X}) - F_c(\boldsymbol{Y}) \ \ s.t. \ \ v^{\boldsymbol{Y}} = v^{\boldsymbol{X}} \right\},$$

and the optima above are achieved when $v = v^{\boldsymbol{X}}$ and $\boldsymbol{Y} = \texttt{Rectflow}(\boldsymbol{X})$.

Proof. Let $\text{var}_c(\dot{X}_t \mid X_t) := \mathbb{E}[c(\dot{X}_t) - c(\mathbb{E}[\dot{X}_t|X_t]) \mid X_t]$. For any v, we have

$$\tilde{L}_{\boldsymbol{X},c}(v) = \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(v(X_t)) - (\dot{X}_t - v(X_t))\nabla c(v(X_t))]\mathrm{d}t$$

$$= \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(v(X_t)) - (v^{\boldsymbol{X}}(X_t) - v(X_t))\nabla c(v(X_t))]\mathrm{d}t \quad //v^{\boldsymbol{X}}(X_t) = \mathbb{E}[\dot{X}_t|X_t]$$

$$\geq \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(v^{\boldsymbol{X}}(X_t))]\mathrm{d}t \quad //c(v^{\boldsymbol{X}}) \geq c(v) + (v^{\boldsymbol{X}} - v)\nabla c(v)$$

$$= \int_0^1 \text{var}_c(\dot{X}_t \mid X_t)\mathrm{d}t,$$

The inequality is tight when $v = v^{\boldsymbol{X}}$, which attains the minimum of $\tilde{L}_{\boldsymbol{X},c}$.

Write $R_{\boldsymbol{X},c}(\boldsymbol{Y}) = F_c(\boldsymbol{X}) - F_c(\boldsymbol{Y})$. We know that $\boldsymbol{Z} = \texttt{Rectify}(\boldsymbol{X})$ attains the maximum of $R_{\boldsymbol{X},c}(\boldsymbol{Y})$ subject to $v^{\boldsymbol{Y}} = v^{\boldsymbol{X}}$ by Lemma 3.3. In addition,

$$R_{\boldsymbol{X},c}(\boldsymbol{Z}) = \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(\dot{Z}_t)]\mathrm{d}t$$

$$= \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(v_t^{\boldsymbol{X}}(Z_t)])]\mathrm{d}t$$

$$= \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(v_t^{\boldsymbol{X}}(X_t)])]\mathrm{d}t \quad //\text{Law}(Z_t) = \text{Law}(X_t), \forall t$$

$$= \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(\mathbb{E}[\dot{X}_t|X_t])]\mathrm{d}t$$

$$= \int_0^1 \mathbb{E}[\text{var}_c(\dot{X}_t \mid X_t)]\mathrm{d}t.$$

This concludes the proof. □

Straight couplings The $\tilde{\ell}^*_{\boldsymbol{X},c} = \int_0^1 \text{var}_c(\dot{X}_t|X_t)\mathrm{d}t$ above provides a measure of how much the different paths of $\boldsymbol{X}$ intersect with each other. If c is strictly convex and $\tilde{\ell}^*_{\boldsymbol{X},c} = 0$, we have $\dot{X}_t = \mathbb{E}[\dot{X}_t|X_t]$ almost surely, meaning that there exist no two paths that go across a point along two different directions. In this case, $\boldsymbol{X}$ is a fixed point of $\texttt{Rectflow}(\cdot)$, that is, $\boldsymbol{X} = \boldsymbol{Z} = \texttt{Rectify}(\boldsymbol{X})$, because we have $\mathrm{d}X_t = \dot{X}_t\mathrm{d}t = \mathbb{E}[\dot{X}_t|X_t]\mathrm{d}t = v^{\boldsymbol{X}}(X_t)\mathrm{d}t$, which is the same Equation (15) that defines $\boldsymbol{Z}$.

Similarly, if $\boldsymbol{X}$ is the linear interpolation of the coupling (X_0, X_1), then $\tilde{\ell}^*_{\boldsymbol{X},c} = 0$ with strictly convex c if and only if (X_0, X_1) is a fixed point of the Rectify mapping, that is, $(X_0, X_1) = \text{Rectify}((X_0, X_1))$, following [LGL22]. Such couplings are called *straight*, or *fully rectified* in [LGL22]. Obtaining straight couplings is useful for learning fast ODE models because the trajectories of the associated rectified flow $\boldsymbol{Z}$ are straight lines and hence can be calculated in closed form without iterative numerical solvers. See [LGL22] for more discussion.

Moreover, [LGL22] showed that rectifiable c-optimal couplings must be straight. In the one dimensional case ($d = 1$), the straight coupling, if it exists, is unique and attains the minimum of $\mathbb{E}[c(X_1 - X_0)]$ for all convex functions for which c-optimal coupling exists. For higher dimensions ($d \geq 2$), however, straight couplings are not unique, and the specific straight coupling obtained at the convergence of the recursive Rectify update (i.e. $(Z_0^{k+1}, Z_1^{k+1}) = \text{Rectify}((Z_0^k, Z_1^k))$) is implicitly determined by the initial coupling (Z_0^0, Z_1^0), and is not expected to be optimal w.r.t. any pre-fixed c.

The following counter example shows a somewhat stronger negative result: there exist straight couplings that are not optimal w.r.t. all second order differentiable convex functions with invertible Hessian matrices.

Example 3.5. *Take $\pi_0 = \pi_1 = \mathcal{N}(0, I)$. Hence, for $c(x) = \|x\|^p$ with $p > 0$, the c-optimal mapping is the trivial identity coupling (X_0, X_0) with $X_0 \sim \pi_0$.*

However, consider the coupling (X_0, AX_0), where A is a non-identity and non-reflecting rotation matrix (namely $A^\top A = I$, $\det(A) = 1$, $A \neq I$ and A does not have $\lambda = -1$ as an eigenvalue). Then (X_0, AX_0) is a straight coupling of π_0 and π_1, but it is not c-optimal for all second order differentiable convex function c whose Hessian matrix is invertible everywhere. See Appendix for the proof.

It is the rotation transform that makes (X_0, AX_0) sub-optimal, which is removed in the proposed c-rectified flow in Section 5 via a Helmholtz like decomposition.

4 Differentiable Processes with Equivalent Marginal Laws

The marginal preserving property of rectified flow is due to the property of $v^{\boldsymbol{Z}} = v^{\boldsymbol{X}}$ by construction. However, we show in this section that $v^{\boldsymbol{X}} = v^{\boldsymbol{Z}}$ is only a sufficient condition: two differentiable processes $\boldsymbol{X}$ and $\boldsymbol{Z}$ can have the same marginal laws even if $r := v^{\boldsymbol{X}} - v^{\boldsymbol{Z}} \neq 0$. This is because r, as illustrated in Example 3.5, can be a rotation-only vector field (in a generalized sense shown below) that introduces rotation components into the dynamics without modifying the marginal distributions. Therefore, the constraint of $v^{\boldsymbol{Y}} = v^{\boldsymbol{X}}$ in the optimization problem (16) may be too restrictive. A natural relaxation of (16) would be

$$\inf_{\boldsymbol{Y}} \left\{ F_c(\boldsymbol{Y}) := \mathbb{E}\left[\int_0^1 c(\dot{Y}_t)\mathrm{d}t\right], \quad s.t. \quad \text{Law}(Y_t) = \text{Law}(X_t), \ \forall t \in [0, 1] \right\}, \tag{17}$$

which yields a dynamic OT problem with a continuum of marginal constraints. In Section 5, we show that the solution of (17) yields our c-rectified flow that solve the OT problem at the fixed point. Solving (17) allows us to remove the rotational components of $v^{\boldsymbol{X}}$, which is what what renders rectified flow non-optimal. In this section, we first characterize the necessary and sufficient condition for having equivalent marginal laws.

Definition 4.1. *A time-dependent vector field $r \colon \mathbb{R}^d \times [0, 1] \to \mathbb{R}^d$ is said to be $\boldsymbol{X}$-marginal-preserving if*

$$\int_0^t \mathbb{E}[\nabla h(X_t)^\top r_t(X_t)] = 0, \quad \forall t \in [0, 1], \quad h \in C_c^1(\mathbb{R}^d). \tag{18}$$

Equation (18) is equivalent to saying that $\mathbb{E}[\nabla h(X_t)^\top r_t(X_t)] = 0$ holds almost surely assuming that t is a random variable following $\mathrm{Uniform}([0,1])$ (i.e., t-almost surely). Let $\rho_t = \mathrm{Law}(X_t)$ and it yields a density function ϱ_t. Using integration by parts, we have

$$0 = \mathbb{E}[\nabla h(X_t)^\top r_t(X_t)] = \int \nabla h(x)^\top r_t(x) \varrho_t(x) \mathrm{d}x = -\int h(x) \nabla \cdot (r_t(x)\varrho_t(x)) \mathrm{d}x, \quad \forall h \in C_c^1(\mathbb{R}^d),$$

which gives $\nabla \cdot (r_t \varrho_t) = 0$. This says that $r_t \varrho_t$ is a rotation-only (or divergence-free) vector field in the classical sense.

Lemma 4.2. *Let X and Y be two stochastic processes with the same initial distributions $\mathrm{Law}(X_0) = \mathrm{Law}(Y_0)$. Assume that X is rectifiable, and $v_t^Y(z) := \mathbb{E}[\dot{Y}_t | Y_t = z]$ exists and is locally bounded.*

Then X and Y share the same marginal laws at all time, that is, $\mathrm{Law}(X_t) = \mathrm{Law}(Y_t)$, $\forall t \in [0,1]$, if and only if $v^X - v^Y$ is Y-marginal-preserving.

Proof. Taking any h in $C_c^1(\mathbb{R}^d)$, we have for $t \in [0,1]$

$$
\begin{aligned}
\mathbb{E}[h(X_t)] - \mathbb{E}[h(X_0)] &= \int_0^t \mathbb{E}[\nabla h(X_s)^\top \dot{X}_s] \mathrm{d}s \\
&= \int_0^t \mathbb{E}[\nabla h(X_s)^\top v_s^X(X_s)] \mathrm{d}s \quad /\!/ v_s^X(X_s) = \mathbb{E}[\dot{X}_s | X_s].
\end{aligned}
$$

This suggests that the marginal law $\rho_t := \mathrm{Law}(X_t)$ satisfies

$$\rho_t(h) - \rho_0(h) - \int_0^t \rho_s(\nabla h^\top v_s^X) \mathrm{d}s = 0, \quad \forall h \in C_c^1(\mathbb{R}^d), \tag{19}$$

where we define $\rho_t(h) = \int h(x) \mathrm{d}\rho_t(x)$. Equation (19) is formally written as the continuity equation:

$$\dot{\rho}_t + \nabla \cdot (g_t^X \rho_t) = 0. \tag{20}$$

Similarly, $\tilde{\rho}_t := \mathrm{Law}(Y_t)$ satisfies

$$\tilde{\rho}_t(h) - \tilde{\rho}_0(h) - \int_0^t \tilde{\rho}_s(\nabla h^\top v_s^Y) \mathrm{d}s = 0, \quad \forall h, \tag{21}$$

If $v_t^X - v_t^Y$ is $\mathrm{Law}(Y_t)$-preserving for $\forall t \in [0,1]$, we have

$$
\begin{aligned}
\mathbb{E}[h(Y_t)] - \mathbb{E}[h(Y_0)] &= \int_0^t \mathbb{E}[\nabla h(Y_s)^\top \dot{Y}_s] \mathrm{d}s \\
&= \int_0^t \mathbb{E}[\nabla h(Y_s)^\top v_s^Y(Y_s)] \mathrm{d}s \\
&= \int_0^t \mathbb{E}[\nabla h(Y_s)^\top v_s^X(Y_s)] \mathrm{d}s + \int_0^t \mathbb{E}[\nabla h(Y_s)^\top (v_s^Y(Y_s) - v_s^X(Y_s))] \mathrm{d}s \\
&= \int_0^t \mathbb{E}[\nabla h(Y_s)^\top v_s^X(Y_s)] \mathrm{d}s \quad /\!/ v^X - v^Y \text{ is } Y\text{-preserving},
\end{aligned}
$$

which suggests that $\tilde{\rho}_t := \mathrm{Law}(Y_t)$ solves the same continuity equation (20), starting from the same initialization as $\mathrm{Law}(X_0) = \mathrm{Law}(Y_0)$. Hence, we have $\rho_t = \tilde{\rho}_t$ if the solution of (20) is unique, which is equivalent to the uniqueness of the solution of $\mathrm{d}Z_t = v_t^{\boldsymbol{X}}(Z_t)$ in (15) following Corollary 1.3 of [Kur11].

On the other hand, if $\rho_t = \mathrm{Law}(X_t) = \mathrm{Law}(Y_t) = \tilde{\rho}_t$, following (19) and (21), we have for any $h \in C_{\mathrm{c}}^1(\mathbb{R}^d)$,

$$0 = \int_0^t \tilde{\rho}_t(\nabla h^\top v_s^{\boldsymbol{X}}) - \tilde{\rho}_t(\nabla h^\top v_s^{\boldsymbol{Y}})\mathrm{d}s = \int_0^t \nabla h(Y_s)^\top(v^{\boldsymbol{X}}(Y_s) - v^{\boldsymbol{Y}}(Y_s))\mathrm{d}s,$$

which is the definition of $\boldsymbol{Y}$-marginal-preserving following (18).

$\square$

5 c-Rectified Flow

We introduce c-rectified flow, a c-dependent variant of rectified flow that guarantees to minimize the c-transport cost when applied recursively. This section is organized as follows: Section 5.1 defines and discusses the c-rectified flow of a differentiable stochastic process $\boldsymbol{X}$, which we show yields the solution of the infinite-marginal OT problem (17). Section 5.2 considers the c-rectified flow of a coupling (X_0, X_1), which we show is non-increasing on the c-transport cost. Section 5.3 proves that the fixed points of c-$\mathtt{Rectify}$ are c-optimal. Section 5.4 interprets c-rectified flow as an alternating direction descent method for the dynamic OT problem (8), and a majorize-minimization (MM) algorithm for the static OT problem (1). Section 5.5 discusses a key lemma relating c-optimal couplings and its associated displacement interpolation with Hamilton-Jacobi equation.

5.1 c-Rectified Flow of Time-Differentiable Processes X

For a convex cost function $c\colon \mathbb{R}^d \to \mathbb{R}$ and a time-differentiable process $\boldsymbol{X}$, the c-rectified flow of $\boldsymbol{X}$, denoted as $\boldsymbol{Z} = c\text{-}\mathtt{Rectflow}(\boldsymbol{X})$, is defined as the solution of

$$\mathrm{d}Z_t = g_t^{\boldsymbol{X},c}(Z_t)\mathrm{d}t, \quad Z_0 = X_0, \quad \text{with} \quad g_t^{\boldsymbol{X},c}(z) = \nabla c^*(\nabla f_t^{\boldsymbol{X},c}(z)), \quad t \in [0,1], \tag{22}$$

where $c^*(x) := \sup_y\{x^\top y - c(y)\}$ is the convex conjugate of c, and $f^{\boldsymbol{X},c}\colon \mathbb{R}^d \times [0,1] \to \mathbb{R}$ is the optimal solution of

$$\inf_f \left\{ L_{\boldsymbol{X},c}(f) := \int_0^1 \mathbb{E}\left[\mathsf{m}_c\left(\dot{X}_t;\ \nabla f_t(X_t) \right) \right] \mathrm{d}t \right\}, \tag{23}$$

where $\mathsf{m}_c : \mathbb{R}^d \times \mathbb{R}^d \to [0, +\infty)$ is a loss function defined as

$$\mathsf{m}_c(x; y) = c(x) - x^\top y + c^*(y).$$

Note that we have $\mathsf{m}_c(x; y) \geq 0$ for $\forall x, y$ following the definition of the conjugate c^* (or the Fenchel-Young inequality). Losses of form $\mathsf{m}_c(x; y)$ is equivalent to the so called *matching loss* proposed for learning generalized linear models [AHW95].

Compared with the original rectified flow, the difference of c-rectified flow is i) restricting the velocity field to a form of $g_t = \nabla c^* \circ \nabla f_t$, and ii) replacing the quadratic objective function to the matching loss. These two changes combined yield a Helmholtz like decomposition of $v^{\boldsymbol{X}}$ as we show below, allowing us to remove the "rotation-only" component of $v^{\boldsymbol{X}}$ and obtain c-optimal couplings at fixed points.

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Bregman divergence, Helmholtz decomposition, marginal preserving We can equivalently write (23) using Bergman divergence associated with c, that is,

$$\mathsf{b}_c(x; y) := c(x) - c(y) - \nabla c(y)^\top (x - y).$$

Then it is easy to see that $\mathsf{m}_c(x; y) = \mathsf{b}_c(x; \nabla c^*(y))$, by using the fact that $\nabla c(\nabla c^*(y)) = y$ and $c^*(y) = y^\top \nabla c^*(y) - c(\nabla c^*(y))$. Hence, m_c and b_c are equivalent up to the monotonic transform ∇c^* on y. The minimum $\mathsf{b}_c(x; y) = 0$ is achieved when $y = x$, while $\mathsf{m}_c(x; y) = 0$ is achieved when $\nabla c^*(y) = x$.

Therefore, (23) is equivalent to

$$\inf_f \int_0^1 \mathbb{E}\left[\mathsf{b}_c\left(\dot{X}_t; \ g_t(X_t)\right)\right] \mathrm{d}t, \qquad \text{with} \quad g_t = \nabla c^* \circ \nabla f_t. \tag{24}$$

Moreover, the generalized Pythagorean theorem of Bregman divergence (e.g., [BMD$^+$05]) gives

$$\mathbb{E}\left[\mathsf{b}_c\left(\dot{X}_t; \ g_t\right) \mid X_t\right] = \mathsf{b}_c\left(\mathbb{E}\left[\dot{X}_t | X_t\right]; \ g_t\right) + \mathbb{E}\left[\mathsf{b}_c\left(\dot{X}_t; \ \mathbb{E}\left[\dot{X}_t | X_t\right]\right)\right]. \tag{25}$$

Because $v^{\boldsymbol{X}}(X_t) = \mathbb{E}\left[\dot{X}_t | X_t\right]$ and the last term of (25) is independent with g_t, we can further reframe (23) into

$$\min_f \int_0^1 \mathbb{E}\left[\mathsf{b}_c\left(v_t^{\boldsymbol{X}}(X_t); \ g_t(X_t)\right)\right] \mathrm{d}t, \qquad \text{with} \quad g_t = \nabla c^* \circ \nabla f_t, \tag{26}$$

which can be viewed as projecting the expected velocity $v_t^{\boldsymbol{X}}$ to the set of functions of form $g_t = \nabla c^* \circ \nabla f_t$, w.r.t. the Bregman divergence. This yields an orthogonal decomposition of $v_t^{\boldsymbol{X}}$:

$$v_t^{\boldsymbol{X}} = \nabla c^* \circ \nabla f_t^{\boldsymbol{X},c} + r_t^{\boldsymbol{X},c}, \tag{27}$$

where $r_t^{\boldsymbol{X},c} = v_t^{\boldsymbol{X},c} - \nabla c^* \circ \nabla f_t^{\boldsymbol{X},c}$ is the residual term. The key result below shows that $r^{\boldsymbol{X},c}$ is $\boldsymbol{X}$-marginal-preserving, which ensures that the c-rectified flow preserves the marginals of $\boldsymbol{X}$.

Definition 5.1. *We say that $\boldsymbol{X}$ is c-rectifiable if $v^{\boldsymbol{X}}$ exists, the minimum of (23) exists and is attained by a locally bounded function $f^{\boldsymbol{X},c}$, and the solution of Equation (22) exists and is unique.*

Theorem 5.2. *Assume that $\boldsymbol{X}$ is c-rectifiable, and $c^* := \sup_y\{x^\top y - c(y)\}$ and $c^* \in C^1(\mathbb{R}^d)$. We have*

i) $v^{\boldsymbol{X}} - g^{\boldsymbol{X},c}$ is $\boldsymbol{X}$-marginal-preserving.

ii) $\boldsymbol{Z} = c\text{-}\mathtt{Rectify}(\boldsymbol{X})$ preserves the marginal laws of $\boldsymbol{X}$, that is, $\mathrm{Law}(Z_t) = \mathrm{Law}(X_t)$, $\forall t \in [0, 1]$.

Proof. i) By $v_t^{\boldsymbol{X}}(z) = \mathbb{E}[\dot{X}_t | X_t = z]$, the loss function in (23) is equivalent to

$$L_{\boldsymbol{X},c}(f) = \int_0^1 \mathbb{E}\left[c^*(\nabla f_t(X_t)) - \mathbb{E}[\dot{X}_t \mid X_t]^\top \nabla f_t(X_t) + c(\dot{X}_t)\right] \mathrm{d}t$$

$$= \int_0^1 \mathbb{E}\left[c^*(\nabla f_t(X_t)) - v_t^{\boldsymbol{X}}(X_t)^\top \nabla f_t(X_t) + c(\dot{X}_t)\right] \mathrm{d}t.$$

By Euler-Lagrange equation, we have

$$\int_0^1 \mathbb{E}\left[(\nabla c^*(\nabla f_s^{\boldsymbol{X},s}(X_s)) - v^{\boldsymbol{X}}(X_s))^\top \nabla g_s(X_s)\right] \mathrm{d}s = 0, \quad \forall g : g_s \in C_{\mathrm{c}}^1(\mathbb{R}^d).$$

Taking $g_s = h$ if $s < t$ and $g_s = 0$ if $s > t$ yields that $r^{\boldsymbol{X},c}(x) = \nabla c^*(\nabla f_s^{\boldsymbol{X},c}(X_s)) - v^{\boldsymbol{X}}(X_s)$ is $\boldsymbol{X}$-marginal-preserving following (18).

ii) Note that $\boldsymbol{Z}$ is rectifiable if $\boldsymbol{X}$ is c-rectifiable. Applying Lemma 4.2 yields the result. □

For the quadratic cost $c(x) = c^*(x) = \frac{1}{2}\|x\|^2$, the ∇c^* is the identity mapping, and (27) reduces to the Helmholtz decomposition, which represents a velocity field into the sum of a gradient field and a divergence-free field. Hence, (27) yields a generalization of Helmholtz decomposition, in which a monotonic transform ∇c^* is applied on the gradient field component. We call (27) a *Bregman Helmholtz decomposition.*

Remark: score matching In some special cases, $v^{\boldsymbol{X}}$ may already be a gradient field, and hence the rectified flow and c-rectified flow coincide for $c(x) = \frac{1}{2}\|x\|^2$. One example of this is when $X_t = \alpha_t X_1 + \beta_t \xi$ for some time-differentiable functions α_t and β_t, and $\xi \sim \mathcal{N}(0, I)$, satisfying $\alpha_1 = 1, \beta_1 = 0$, and $X_0 = \alpha_0 X_1 + \beta_0 \xi$. In this case, one can show that

$$v_t^{\boldsymbol{X}}(z) = \mathbb{E}[\dot{\alpha}_t X_1 + \dot{\beta}_t X_0 \mid X_t = z] = \nabla f_t(z), \qquad \text{with} \qquad f_t(z) = \eta_t \log \varrho_t(z) + \frac{\zeta_t}{2}\|z\|^2,$$

where ϱ_t is the density function of X_t with $\varrho_t(z) \propto \int \phi\left(\frac{z - \alpha_t x_1}{\beta_t}\right) \mathrm{d}\pi_1(x_1)$ and $\phi(z) = \exp(-\|z\|^2/2)$, and $\eta_t = \beta_t^2(\dot{\alpha}_t/\alpha_t - \dot{\beta}_t/\beta_t)$ and $\zeta_t = \dot{\alpha}_t/\alpha_t$. This case covers the probability flow ODEs [SSDK$^+$20] and denoising diffusion implicit models (DDIM) [SME20] with different choices of α_t and β_t as suggested in [LGL22]. When $\zeta_t = 0$, as the case of [SE19], $v_t^{\boldsymbol{X}}$ is proportional to $\nabla \log \rho_t$, the *score function* of ϱ_t, and the least squares loss $L_{\boldsymbol{X}}(v)$ in (12) reduces to a time-integrated *score matching* loss [HD05, Vin11].

However, $v_t^{\boldsymbol{X}}$ is generally not a score function or gradient function, especially in complicate cases when the coupling (X_0, X_1) is induced from the previous rectified flow as we iteratively apply the rectification procedure. In these cases, it is necessary to impose the gradient form as we do in c-rectified flow.

c-**Rectified flow solves Problem** (17) We are ready to show that the c-rectified flow solves the optimization problem in (17). Further, (23) forms a dual problem of (17).

Theorem 5.3. *Under the conditions in Theorem 5.2, we have*

i) $\boldsymbol{Z} = c\text{-}\mathtt{Rectify}(\boldsymbol{X})$ *attains the minimum of* (17).

ii) Problem (17) *and* (23) *has a strong duality:*

$$\inf_f L_{\boldsymbol{X},c}(f) = \sup_{\boldsymbol{Y}} \left\{F_c(\boldsymbol{X}) - F_c(\boldsymbol{Y}) : \mathrm{Law}(Y_t) = \mathrm{Law}(X_t), \ \forall t \in [0,1]\right\}.$$

As the optima above are achieved by $f^{\boldsymbol{X},c}$ *and* $\boldsymbol{Z}$*, we have* $L_{\boldsymbol{X},c}(f^{\boldsymbol{X},c}) = F_c(\boldsymbol{X}) - F_c(\boldsymbol{Z})$.

Proof. Write $R_{\boldsymbol{X},c}(\boldsymbol{Y}) = F_c(\boldsymbol{X}) - F_c(\boldsymbol{Y})$. First, we show that $L_{\boldsymbol{X},c}(f) \geq R_{\boldsymbol{X},c}(\boldsymbol{Y})$ for any f and $\boldsymbol{Y}$ that satisfies $\mathrm{Law}(Y_t) = \mathrm{Law}(X_t), \forall t$:

$$R_{\boldsymbol{X},c}(\boldsymbol{Y})$$

$$= \mathbb{E}\left[\int_0^1 c(\dot{X}_t) - c(\dot{Y}_t)\mathrm{d}t\right]$$

$$\overset{(1)}{\leq} \mathbb{E}\left[\int_0^1 c(\dot{X}_t) + c^*(\nabla f_t(Y_t)) - \dot{Y}_t^\top \nabla f_t(Y_t)\mathrm{d}t\right] \qquad \textcolor{magenta}{\text{//Fenchel-Young inequality: } c(y) \geq x^\top y - c^*(x)}$$

$$= \mathbb{E}\left[\int_0^1 c(\dot{X}_t) + c^*(\nabla f_t(Y_t)) - v_t^{\boldsymbol{Y}}(Y_t)^\top \nabla f_t(Y_t)\mathrm{d}t\right] \quad \textcolor{magenta}{\text{//}v_t^{\boldsymbol{Y}}(Y_t) = \mathbb{E}[\dot{Y}_t|Y_t]}$$

$$= \mathbb{E}\left[\int_0^1 c(\dot{X}_t) + c^*(\nabla f_t(X_t)) - v_t^{\boldsymbol{Y}}(X_t)^\top \nabla f_t(X_t)\mathrm{d}t\right] \quad \textcolor{magenta}{\text{//Law}(X_t) = \mathrm{Law}(Y_t)}$$

$$= \mathbb{E}\left[\int_0^1 c(\dot{X}_t) + c^*(\nabla f_t(X_t)) - v_t^{\boldsymbol{X}}(X_t)^\top \nabla f_t(X_t)\mathrm{d}t\right] \quad \textcolor{magenta}{\text{//}v^{\boldsymbol{X}} - v^{\boldsymbol{Y}} \text{ is } \boldsymbol{X}\text{-marginal-preserving}}$$

$$= L_{\boldsymbol{X},c}(f).$$

Moreover, if we take $\boldsymbol{Y} = \boldsymbol{Z}$ and $f = f^{\boldsymbol{X},c}$, then the inequality in $\overset{(1)}{\leq}$ is tight because $\dot{Z}_t = \nabla c^*(\nabla f_t(Y_t))$ holds t-almost surely. Therefore, $R_{\boldsymbol{X},c}(\boldsymbol{Z}) = L_{\boldsymbol{X},c}(f^{\boldsymbol{X},c}) \geq R^{\boldsymbol{X},c}(Y)$, which suggests that $\boldsymbol{Z}$ attains the maximum of $R_{\boldsymbol{X},c}$ (under the marginal constraints) and the strong duality holds. $\square$

5.2 c-Rectified Flow of Coupling (X_0, X_1)

Similar to the case of rectified flow, the c-rectified flow/coupling of a coupling (X_0, X_1) is defined as the c-rectified flow/coupling of its linear interpolation process. In the following, we show that the c-rectified coupling of a coupling yields no larger c-transport cost.

Definition 5.4. *Let $\boldsymbol{X}$ be the linear interpolation of coupling (X_0, X_1) in that $X_t = tX_1 + (1-t)X_0, \forall t \in [0,1]$. We say that (X_0, X_1) is c-rectifiable if $\boldsymbol{X}$ is c-rectifiable, and call $\boldsymbol{Z} = c\text{-Rectflow}(\boldsymbol{X})$ the c-rectified flow of (X_0, X_1). We call the induced (Z_0, Z_1) the c-rectified coupling of (X_0, X_1), denoted as $(Z_0, Z_1) = c\text{-Rectify}((X_0, X_1))$.*

Note that the c-transport cost $\mathbb{E}[c(X_1 - X_0)]$ is related to the path-wise c-transport cost $F_c(\boldsymbol{X})$ via

$$F_c(\boldsymbol{X}) = \mathbb{E}[c(X_1 - X_0)] + S_c(\boldsymbol{X}), \qquad S_c(\boldsymbol{X}) := \int_0^1 \mathbb{E}[c(\dot{X}_t) - c(X_1 - X_0)]\mathrm{d}t,$$

where $S_c(\boldsymbol{X})$ is a non-negative measurement of how close $\boldsymbol{X}$ is to be geodesic: We have $S_c(\boldsymbol{X}) \geq 0$ following Jensen's inequality $\int_0^1 c(\dot{X}_t)\mathrm{d}t \geq c(\int_0^1 \dot{X}_t \mathrm{d}t) = c(X_1 - X_0)$, and $S_c(\boldsymbol{X}) = 0$ if $X_t = tX_1 + (1-t)X_0$.

Hence, when $\boldsymbol{X}$ is the linear interpolation of (X_0, X_1), we have from Theorem 5.3 that

$$\mathbb{E}[c(X_1 - X_0)] - \mathbb{E}[c(Z_1 - Z_0)] = S_c(\boldsymbol{Z}) + L_{\boldsymbol{X},c}(f^{\boldsymbol{X},c}) \geq 0. \tag{28}$$

which establishes that (Z_0, Z_1) yields no larger transport cost than (X_0, X_1).

Theorem 5.5. *Assume that c is convex with conjugate $c^* \in C^1(\mathbb{R}^d)$, and the conditions in Definition 5.4 holds. Then Equation (28) holds and $\mathbb{E}[c(Z_1 - Z_0)] \leq \mathbb{E}[c(X_1 - X_0)]$.*

Compared with the regular `Rectify` mapping, the key difference here is that the monotonicity of c-`Rectify` only holds for the specific c that it employees, rather than all convex cost functions. More importantly, as we show below, recursively applying c-`Rectify` yields optimal couplings w.r.t. c, a key property that the regular rectified flow misses.

5.3 Fixed Points of c-`Rectify` are c-Optimal

We show three key results regarding the optimality of fixed points of the c-`Rectify` mapping:

1) A coupling (X_0, X_1) is a fixed point of c-`Rectify`, that is, $(X_0, X_1) = c$-`Rectify`$((X_0, X_1))$, if and only if it is c-optimal;

2) Define $\ell^*_{X,c} = \inf_f L_{X,c}(f)$ where X is the linear interpolation of (X_0, X_1). Then $\ell^*_{X,c}$ yields an indication of c-optimality of (X_0, X_1), that is, $L^*_{X,c} = 0$, iff (X_0, X_1) is c-optimal.

3) The minimum $\ell^*_{X,c}$ in the first k iterations of c-`Rectify` steps decreases with an $O(1/k)$ rate.

Theorem 5.6. *Assume that c is convex with conjugate c^*, and $c, c^* \in C^1(\mathbb{R}^d)$ and X is the linear interpolation process of (X_0, X_1). Assume that (X_0, X_1) is a c-rectifiable coupling, and $f^{X,c} \in C^{2,1}(\mathbb{R}^d \times [0, 1])$. Then the following statements are equivalent:*

i) (X_0, X_1) is a fixed point of c-`Rectify`, that is, $(X_0, X_1) = c$-`Rectify`(X_0, X_1).

ii) $\ell^*_{X,c} := \inf_f L_{X,c}(f) = L_{X,c}(f^{X,c}) = 0$, for $L_{X,c}$ in (23).

iii) (X_0, X_1) is a c-optimal coupling.

Proof. i) $\to$ ii). If $(Z_0, Z_1) = (X_0, X_1)$, we have $S_c(Z) = 0$ and $L_{X,c}(f^{X,c}) = 0$ following (28).

iii) $\to$ ii). If (X_0, X_1) is c-optimal, we have $\mathbb{E}[c(X_1 - X_0)] \leq \mathbb{E}[c(Z_1 - Z_0)]$, which again implies that $L_{X,c}(f^{X,c}) = 0$ following (28).

ii) $\to$ i) Note that

$$L_{X,c}(f^{X,c}) = \int_0^1 \mathbb{E}\left[b_c\left(\dot{X}_t;\ g_t^{X,c}(X_t) \right) \right] dt \geq 0.$$

Therefore, $L_{X,c}(f^{X,c}) = 0$ implies that $\dot{X}_t = g_t^{X,c}(X_t)$ t-almost surely. Because Z_t satisfies the same equation, whose solution is assumed to be unique, we have $Z = X$ and hence $(Z_0, Z_1) = (X_0, X_1)$.

ii) $\to$ iii) Because X is the linear interpolation, we have $X_t = tX_1 + (1 - t)X_0$, and it simultaneously satisfies the ODE $dX_t = g_t^{X,c}(X_t)dt$. Using Lemma 5.9 shows that (X_0, X_1) is c-optimal. $\qquad\square$

Knowing that $L_{X,c}(f^{X,c})$ is an indication of c-optimality, we show below that it is guaranteed to converge to zero with recursive `Rectify` updates.

Corollary 5.7. *Let Z^k be the k-th c-rectified flow of (X_0, X_1), satisfying $Z^{k+1} = c$-`Rectflow`$((Z_0^k, Z_1^k))$ and $(Z_0^0, Z_1^0) = (X_0, X_1)$. Assume each (Z_0^k, Z_1^k) is c-rectifiable for $k = 0, \ldots, K$. Then*

$$\sum_{k=0}^K L_{Z^k,c}(f^{Z^k,c}) + S_c(Z^{k+1}) \leq \mathbb{E}[c(X_1 - X_0)].$$

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Therefore, if $\mathbb{E}[c(X_1 - X_0)] < +\infty$, *we have* $\min_{k \leq K} L_{\boldsymbol{Z}^k,c}(f^{\boldsymbol{Z}^k,c}) + S_c(\boldsymbol{Z}^{k+1}) = O(1/K)$.

Proof. Applying (28) to (Z_0^k, Z_1^k) and (Z_0^{k+1}, Z_1^{k+1}) yields

$$L_{\boldsymbol{Z}^k,c}(f^{\boldsymbol{Z}^k,c}) + S_c(\boldsymbol{Z}^{k+1}) = \mathbb{E}[c(Z_1^k - Z_0^k)] - \mathbb{E}[c(Z_1^{k+1} - Z_0^{k+1})].$$

Summing it over $k = 0, \ldots, K$,

$$\sum_{k=0}^{K} L_{\boldsymbol{Z}^k,c}(f^{\boldsymbol{Z}^k,c}) + S_c(\boldsymbol{Z}^{k+1}) = \sum_{k=0}^{K} \mathbb{E}[c(Z_1^k - Z_0^k)] - \mathbb{E}[c(Z_1^{k+1} - Z_0^{k+1})]$$
$$= \mathbb{E}[c(Z_1^0 - Z_0^0)] - \mathbb{E}[c(Z_1^{K+1} - Z_0^{K+1})]$$
$$\leq \mathbb{E}[c(X_1 - X_0)].$$

$\square$

5.4 c-**Rectified Flow as Optimization Algorithms**

In this section, we draw more understanding on how iterative c-rectified flowing solves the static and dynamic OT problems. We first show that c-rectified flow can be viewed as an alternative direction descent on the dynamic OT problem (8), and then that c-rectified coupling as a majorize-minimization (MM) algorithm on the statistic OT problem (1). The results in this section are framed in terms of a general path-wise loss function $F_c(\boldsymbol{Y})$, and hence provide a useful starting point for deriving c-rectified flow like approaches to more general optimization problems with coupling constraints.

c-**Rectified flow as alternative direction descent on** (8)   The mapping $\boldsymbol{Z}^{k+1} = c\text{-Rectflow}(\boldsymbol{Z}^k)$ can be interpreted as an alternative direction descent procedure for the dynamic OT problem (8):

$$\boldsymbol{X}^k = \arg\min_{\boldsymbol{Y}} \left\{ F_c(\boldsymbol{Y}) \quad s.t. \quad (Y_0, Y_1) = (Z_0^k, Z_1^k) \right\}, \tag{29}$$

$$\boldsymbol{Z}^{k+1} = \arg\min_{\boldsymbol{Y}} \left\{ F_c(\boldsymbol{Y}) \quad s.t. \quad \text{Law}(Y_t) = \text{Law}(X_t^k), \ \forall t \in [0,1] \right\}. \tag{30}$$

Here in (29), we minimize $F_c(\boldsymbol{Y})$ in the set of processes whose start-end pair (Y_0, Y_1) equals the coupling (Z_0^k, Z_1^k) from $\boldsymbol{Z}^k$, which simply yields the linear interpolation $X_t^k = tZ_1^k + (1-t)Z_0^k$ by Jensen's inequality. In (30), we minimize $F_c(\boldsymbol{Y})$ given the path-wise marginal constraint of $\text{Law}(Y_t) = \text{Law}(X_t^k)$ for all time $t \in [0,1]$, which yields the c-rectified flow following Theorem 5.3. Note that the updates in both (29) and (30) keep the start-end marginal laws $\text{Law}(Y_0)$ and $\text{Law}(Y_1)$ unchanged, and hence the algorithm stays inside the feasible set $\{\boldsymbol{Y} : \text{Law}(Y_0) = \pi_0, \text{Law}(Y_1) = \pi_1\}$ in (8) once it is initialized to be so.

The updates in (29)-(30) highlight a key difference between our method and the Benamou-Brenier approach (9)-(10): the key idea of Benamou-Brenier is to restrict the optimization domain to the set of deterministic, ODE-induced processes (a.k.a. flows), but our updates alternate between the deterministic c-rectified flow $\boldsymbol{Z}^k$ and the linear interpolation process $\boldsymbol{X}^k$, which is *not* deterministic or ODE-inducable unless the fixed point is achieved.

c-**Rectified flow as an MM algorithm**   The majorize-minimization (MM) algorithm [HL04] is a general optimization recipe that works by finding a surrogate function that *majorizes* the objective function. Let $F(X)$ be the objective concave function to be minimize. An MM algorithm consists of iterative update of form $X^{k+1} \in \arg\min_Y F^+(Y \mid X^k)$, where F^+ is a majorization function of F that satsifies

$$F(Y) = \min_X F^+(Y \mid X), \quad \text{and the minimum is attained when } X = Y.$$

In this case, the MM update guarantees that $F(X^k)$ is monotonically non-increasing:

$$F(X^{k+1}) \le F^+(X^{k+1}|X^k) \le F^+(X^k \mid X^k) = F(X^k).$$

One can also view MM as conducting coordinate descent on (X, Y) for solving $\min_{X,Y} F^+(Y \mid X)$.

In the following, we show that $(Z_0^{k+1}, Z_1^{k+1}) = c\text{-Rectify}((Z_0^k, Z_1^k))$ can be interpreted as an MM algorithm for the static OT problem (1) for minimizing $\mathbb{E}[c(X_1 - X_1)]$ in the set of couplings of π_0 and π_1. The majorization function corresponding to $c\text{-Rectify}$ can be shown to be

$$F_c^+((Y_0, Y_1) \mid (X_0, X_1)) = \inf_{\tilde{\boldsymbol{Y}}} \left\{ F_c(\tilde{\boldsymbol{Y}}) \quad s.t. \quad (\tilde{Y}_0, \tilde{Y}_1) = (Y_0, Y_1), \quad \boldsymbol{Y} \in \mathcal{M}_X \right\},$$

$$\text{with} \quad \mathcal{M}_X = \{\boldsymbol{Y}: \ \text{Law}(Y_t) = \text{Law}(tX_1 + (1-t)X_0), \ \forall t \in [0,1]\},$$

where $F_c^+((Y_0, Y_1) \mid (X_0, X_1))$ denotes the minimum value of $F_c(\tilde{\boldsymbol{Y}})$ for $\tilde{\boldsymbol{Y}}$ whose start-end points equal (Y_0, Y_1), and yields the same marginal laws as that of the linear interpolation process of (X_0, X_1).

Proposition 5.8. *i)* F_c^+ *yields a majorization function of the c-transport cost* $\mathbb{E}[c(Y_1 - Y_0)]$ *in the sense that*

$$\mathbb{E}[c(Y_1 - Y_0)] = \min_{(X_0, X_1)} \{F_c^+((Y_0, Y_1) \mid (X_0, X_1)), \ \ s.t. \ \ (X_0, X_1) \in \Pi_{0,1}\},$$

and the minimum is attained by $(X_0, X_1) = (Y_0, Y_1)$, *where* $\Pi_{0,1}$ *denotes the set of couplings of* π_0 *and* π_1.

ii) $c\text{-Rectify}$ *yields the MM update related* F^+ *in that*

$$c\text{-Rectify}((X_0, X_1)) \in \arg\min_{(Y_0, Y_1) \in \Pi_{0,1}} F_c^+((Y_0, Y_1) \mid (X_0, X_1)).$$

Proof. i) For any coupling (X_0, X_1) and (Y_0, Y_1), we have

$$F_c^+((Y_0, Y_1)|(X_0, X_1)) \ge \inf_{\tilde{\boldsymbol{Y}}} \left\{ \boldsymbol{F}_c(\tilde{\boldsymbol{Y}}) \quad s.t. \quad (\tilde{Y}_0, \tilde{Y}_1) = (Y_0, Y_1) \right\} = \mathbb{E}[c(Y_1 - Y_0)],$$

where the inequality holds because remove the constraint $\boldsymbol{Y} \in \mathcal{M}_X$. In addition, it is obvious that the inequality above becomes equality when $(X_0, X_1) = (Y_0, Y_1)$.

ii) Note that

$$\inf_{(Y_0, Y_1)} F_c^+((Y_0, Y_1) \mid (X_0, X_1)) = \inf_{\boldsymbol{Y}} \{F_c(\boldsymbol{Y}) \quad s.t. \quad \boldsymbol{Y} \in \mathcal{M}_X\},$$

whose minimum of the right side is attained by $\boldsymbol{Y} = c\text{-Rectflow}((X_0, X_1))$ following Theorem 5.3. Hence, the minimum of the left side is attained by $(Y_0, Y_1) = c\text{-Rectify}((X_0, X_1))$. $\square$

5.5 Hamilton-Jacobi Equation and Optimal Transport

The proof of Theorem 5.6 relies on a key lemma shows that if the trajectories of an ODE of form $\mathrm{d}X_t = \nabla c^*(\nabla f_t(X_t))\mathrm{d}t$ are geodesic in that $X_t = tX_1 + (1-t)X_0$, then the induced coupling (X_0, X_1) is an c-optimal coupling of its marginals. The proof of this lemma relies on Hamilton-Jacobi (HJ) equation, which provides a characterization of f for an ODE $\mathrm{d}X_t = \nabla c^*(\nabla f_t(X_t))\mathrm{d}t$ whose trajectories are geodesic. The connection between HJ equation and optimal transport has been a classic result and can be found in, for example, [Vil21, Vil09].

Lemma 5.9. *Let $v_t(x) = \nabla c^*(\nabla f_t(x))$ where $c^* \in C^1(\mathbb{R}^d)$ is a convex function c, and $f \in C^{2,1}(\mathbb{R}^d \times [0,1])$ and ∇c^* is an injective mapping. Assume all trajectories of $\mathrm{d}x_t = v_t(x_t)\mathrm{d}t$ are geodesic paths in that $x_t = tx_1 + (1-t)x_0$. Then we have:*

i) There exists $\tilde{f}_t$ such that $\nabla \tilde{f}_t = \nabla f_t$ (and hence we can replace f with $\tilde{f}$ in the assumption), such that the following Hamilton–Jacobi (HJ) equation holds

$$\partial_t \tilde{f}_t(x) + c^*(\nabla \tilde{f}_t(x)) = 0, \quad \forall x \in \mathbb{R}^d, \ t \in [0,1], \qquad \text{(HJ equation)}. \qquad (31)$$

ii) f satisfies

$$f_t(y_t) = \inf_{y_0 \in \mathbb{R}^d} \left\{ tc\left(\frac{y_t - y_0}{t}\right) + f_0(y_0) \right\}, \quad \forall t \in [0,1], \quad y_t \in \mathbb{R}^d, \qquad \text{(Hopf-Lax formula)}$$

where the minimum is attained if $\{y_t\}$ follows the ODE $\mathrm{d}y_t = v_t(y_t)\mathrm{d}t$.

iii) Assume a coupling (X_0, X_1) of π_0, π_1 satisfies $\mathrm{d}X_t = v_t(X_t)\mathrm{d}t$. Then (X_0, X_1) is a c-optimal coupling.

Proof. i) Starting from any point $x_t = x \in \mathbb{R}^d$ at time t, because the trajectories of $\mathrm{d}x_t = v_t(x_t)\mathrm{d}t$ are geodesic, we have $\dot{x}_t = v_t(x_t) = const$ following the trajectory. Because $v_t(x) = \nabla c^*(\nabla f_t(x))$ and ∇c^* is injective, we have $\nabla f_t(x_t) = const$ as well. Hence, we have

$$\begin{aligned}
0 = \frac{\mathrm{d}}{\mathrm{d}t} \nabla f_t(x_t) &= \partial_t \nabla f_t(x_t) + \nabla^2 f_t(x_t)\dot{x}_t \\
&= \partial_t \nabla f_t(x_t) + \nabla^2 f_t(x_t)\nabla c^*(\nabla f_t(x_t)).
\end{aligned}$$

On the other hand, define $h_t(x) = \partial_t f_t(x) + c^*(\nabla f_t(x))$. Then we have

$$\nabla_x h_t(x) = \partial_t \nabla f_t(x) + \nabla^2 f_t(x_t)\nabla c^*(\nabla f_t(x)) = 0.$$

This suggests that $\nabla_x h_t(x) = 0$ everywhere and hence $h_t(x)$ does not depend on x. Define $\tilde{f}_t(x) = f_t(x) - \int_0^t h_t(x_0)\mathrm{d}t$, where x_0 is any fixed point in $\mathbb{R}^d$. Then

$$\tilde{h}_t(x) := \partial_t \tilde{f}_t(x) + c^*(\nabla \tilde{f}_t(x)) = h_t(x) - h_t(x_0) = 0.$$

ii) Take any y_0, y_1 in $\mathbb{R}^d$, let $y_t = ty_1 + (1-t)y_0$ be their linear interpolation. We have

$$f_1(y_1) - f_0(y_0)$$
$$= \int_0^1 (\partial_t f_t(y_t) + \nabla f_t(y_t)^\top (y_t - y_0))\mathrm{d}t$$
$$= \int_0^1 \nabla f_t(y_t)^\top (y_1 - y_0) - c^*(\nabla f_t(y_t))\mathrm{d}t \qquad /\!/ h_t = \partial f_t + c^*(\nabla f_t) = 0$$
$$\overset{(1)}{\leq} \int_0^1 c(y_1 - y_0)\mathrm{d}t \qquad /\!/ c(x) + c^*(y) \geq x^\top y$$
$$= c(y_1 - y_0).$$

The equality in $\overset{(1)}{\leq}$ is attained if y_t follows the geodesic ODE $\mathrm{d}y_t = v_t(y_t)\mathrm{d}t$ as we have $y_1 - y_0 = \nabla c^*(\nabla f_t(y_t))$, $\forall t$ in this case. A similar derivation holds for f_t.

iii) Note that i) gives that $c(y_1 - y_0) \geq f_1(y_1) - f_0(y_0)$. For any coupling (Y_0, Y_1) of π_0, π_1, we have

$$\mathbb{E}[c(Y_1 - Y_0)] \geq \mathbb{E}[f_1(Y_1) - f_0(Y_0)] = \mathbb{E}[f_1(X_1) - f_0(X_0)] = \mathbb{E}[c(X_1 - X_0)].$$

Hence, (X_0, X_1) is a c-optimal coupling. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Connection to Benamou-Brenier Formula The results in Lemma 5.9 can also formally derived from Benamou-Brenier problem (10), as shown in the seminal work of [BB00]. By introducing a Lagrangian multiplier $\lambda \colon \mathbb{R}^d \times [0,1] \to \mathbb{R}$ for the constraint of $\dot{\varrho}_t + \nabla \cdot (v_t \varrho_t) = 0$, the problem in (10) can be framed into a minimax problem:

$$\inf_{v, \varrho} \sup_\lambda \left\{ \mathcal{L}(v, \varrho, \lambda) := \int c(v_t)\varrho_t + \int \lambda_t(\dot{\varrho}_t + \nabla \cdot (v_t \varrho_t) \quad s.t. \quad \varrho \in \Gamma_{0,1} \right\},$$

where $\mathcal{L}(v, \varrho, \lambda)$ is the Lagrangian function, and $\Gamma_{0,1}$ denotes the set of density functions $\{\varrho_t\}_t$ satisfying $\varrho_0 = \mathrm{d}\pi_0/\mathrm{d}x$, $\varrho_1 = \mathrm{d}\pi_1/\mathrm{d}x$. Note that the following integration by parts formulas:

$$\int \lambda_t \nabla \cdot (v_t \varrho_t) + \nabla \lambda_t^\top v_t \varrho_t = 0, \qquad\qquad \int \lambda_t \dot{\varrho}_t + \dot{\lambda}_t \varrho_t = \lambda_1 \varrho_1 - \lambda_0 \varrho_0,$$

where we assume that $\lambda_t v_r \rho_t$ decays to zero sufficiently fast at infinity. We have

$$\mathcal{L}(v, \varrho, \lambda) = (\lambda_1 \varrho_1 - \lambda_0 \varrho_0) + \int (c \circ v_t)\rho_t - \dot{\lambda}_t \varrho_t - \nabla \lambda_t^\top (v_t \varrho_t).$$

At the saddle points, the functional derivations of $\mathcal{L}$ equal zero, yielding

$$\frac{\delta \mathcal{L}}{\delta \varrho_t} = c(v_t) - \dot{\lambda}_t - \nabla \lambda_t^\top v_t = 0, \qquad\qquad \frac{\delta \mathcal{L}}{\delta v_t} = (\nabla c(v_t) - \nabla \lambda_t)\varrho_t = 0.$$

Assume ϱ_t is positive everywhere and note that $\nabla c^*(\nabla c(x)) = x$, we have $v_t = \nabla c^*(\nabla \lambda_t)$, and hence $\nabla \lambda_t^\top v_t - c(v_t) = c^*(\nabla \lambda_t)$. Plugging it back to $\frac{\delta \mathcal{L}}{\delta \rho_t} = 0$ yields that $\dot{\lambda}_t + c^*(\nabla \lambda_t) = 0$. Overall, the (formal) KKT condition of (10) is

$$\dot{\varrho}_t + \nabla \cdot (v_t \varrho_t) = 0, \quad \rho_0 = \mathrm{d}\pi_0/\mathrm{d}x, \quad \rho_1 = \mathrm{d}\pi_1/\mathrm{d}x \qquad /\!/ \text{coupling condition}$$
$$v_t = \nabla c^*(\nabla \lambda_t) \qquad /\!/ \text{mapping is gradient of convex function}$$
$$\dot{\lambda}_t + c^*(\nabla \lambda_t) = 0. \qquad /\!/ \text{Hamilton-Jacobi equation}$$

This matches the result in Lemma 5.9 with $\lambda_t = \tilde{f}_t$.

6   Discussion and Open Questions

1. Corollary 5.7 only bounds the surrogate measure $\ell^*_{Z^k,c}$. Can we directly bound the optimality gap on the c-transport cost $e^*_k = \mathbb{E}[c(Z^k_1 - Z^k_0)] - \inf_{(Z_0,Z_1)} \mathbb{E}[c(Z_1 - Z_0)]$? Can we find a certain type of strong convexity like condition, under which e^*_k decays exponentially with k?

2. For machine learning (ML) tasks such as generative models and domain transfer, the transport cost is not necessarily the direct object of interest. In these cases, as suggested in [LGL22], rectified flow might be preferred because it is simpler and does not require to specify a particular cost c. Question: for such ML tasks, when would it be preferred to use OT with a specific c, and how to choose c optimally?

3. In practice, recursively applying the $(c$-)rectification accumulates errors because the training optimization for the drift field and the simulation of the ODE can not be conducted perfectly. How to avoid the error accumulation at each step? Assume $\{x_{1,i}\}_i \sim \pi_1$, and $\{z^k_{0,i}, z^k_{1,i}\}_i$ is obtained by solving the ODE of the k-th c-rectified flow starting from $z^k_{0,i} \sim \pi_0$. As we increase k, $\{z^k_{0,i}\}_i$ may yield increasingly bad approximation of π_1 due to the error accumulation. One way to fix this is to adjust $\{z^k_{1,i}\}$ to make it closer to $\{x^k_{1,i}\}_i$ at each step. This can be done by reweighting/transporting $\{z^k_{1,i}\}_i$ towards $\{x^k_{1,i}\}_i$ by minimizing certain discrepancy measure, or replacing each $z^k_{1,i}$ with $x^k_{\sigma(i)}$ where σ is a permutation that yields a one-to-one matching between $\{z^{(i)}_1\}$ and $\{x^{(i)}_1\}_i$. The key and challenging part is to do the adjustment in a good and fast way, ideally with a (near) linear time complexity.

4. With or without the adjustment step, build a complete theoretical analysis on the statistical error of the method.

5. In what precise sense is rectified flow solving a multi-objective variant of optimal transport?

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A   Proofs

Proof of Example 3.5. i) The fact that $A^\top A = I$ and $\pi_0 = \pi_1 = \mathcal{N}(0, I)$ ensures that $AX_0 \sim \pi_1$ and hence (X_0, AX_0) is a coupling of π_0 and π_1. Let $X_t = tAX_0 + (1-t)X_0$ be the linear interpolation of the coupling. Related, we have $\dot{X}_t = AX_0 - X_0$. Canceling X_0 yields that

$$\dot{X}_t = (A - I)(tA + (1-t)I)^{-1}X_t, \tag{32}$$

where we use the fact that $tA + (1-t)I$ is convertible for $t \in [0, 1]$, which we prove as follows: if $tA + (1-t)I$ is not invertible, then A must have $\lambda = -\frac{1-t}{t}$ as one of its eigenvalues; but as a rotation matrix, all eigenvalues of A must have a norm of 1, which means that we must have $t = 0.5$ and $\lambda = -1$. This, however, is excluded by the assumption that A is non-reflecting (and hence $\lambda \neq -1$).

Equation (32) shows that $\dot{X}_t$ is uniquely determined by X_t. Hence, we have $\int_0^1 \mathbb{E}\left[\mathrm{var}(\dot{X}_t|X_t)\right]\mathrm{d}t = 0$, which implies that (X_0, AX_0) is a straight coupling by Theorem 3.6 of [LGL22].

2) Let c be a second order differentiable convex function whose Hessian matrix $\nabla^2 c(x)$ is invertible everywhere. Let c^* be the convex conjugate of c, then c^* is also second order differentiable and $\nabla c(\nabla c^*(x)) = x$, and $\nabla^2 c^*(x) = \nabla^2 c(x)^{-1}$.

If (X_0, AX_0) is a c-optimal coupling, there must exists a function $\phi\colon \mathbb{R}^d \to \mathbb{R}$, such that

$$Ax = x + \nabla c^*(\nabla \phi(x)), \quad \forall x, \tag{33}$$

where c^* is the convex conjugate of c. Equation (33) is equivalent to $\nabla c(Ax - x) = \nabla \phi(x)$, which means that $\nabla \phi$ is continuously differentiable. Taking gradient on both sides of (33) gives

$$A - I = H_x B_x, \qquad\qquad H_x = \nabla^2 c^*(\nabla \phi(x)), \quad B_x = \nabla^2 \phi(x), \tag{34}$$

where H_x, B_x are both symmetric and H_x is positive definite, and hence Then $H_x B_x$ is a diagonalizable (all its eigenvalues are real) by Lemma A.1. However, $A - I$ is not diagonalizable because A must have complex eigenvalues as a non-reflecting, non-identity rotation matrix. Hence, (34) can not hold.

Lemma A.1. *Assume that A, B are two real symmetric matrices and A is positive definite. Then AB is diagonalizable (on the real domain), that is, there exists an invertible matrix P, such that $P^{-1}ABP$ is a diagonal matrix.*

Proof. This is a standard result in linear algebra. Because A is positive definite, there exists an invertible symmetric matrix C, such that $CC = A$. Then, $AB = CCB$, and it is similar to CBC^{-1}, which is symmetric and hence diagonalizable. $\square$

$\square$