

A discrete Benamou-Brenier formulation of Optimal Transport on graphs

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Abstract—We propose a discrete transport equation on graphs which connects distributions on both vertices and edges. We then derive a discrete analogue of the Benamou-Brenier formulation for Wasserstein-1 distance on a graph and as a result classify all W_1 geodesics on graphs.

Index Terms—graph, network, optimal transport, Wasserstein, incidence matrix, Beckmann, Benamou-Brenier, transport equation, geodesics, discrete divergence.

I. INTRODUCTION

The classical transport problem considers two measures μ and ν on spaces \mathcal{X} and \mathcal{Y} , where we have cost (and in our case a metric) of transporting $x \in \mathcal{X}$ to $y \in \mathcal{Y}$, which we denote $d(x, y)$. Then we ask: how can we transport μ to ν while minimising the expected cost? This gives us a measure of discrepancy between μ and ν relative to $d(x, y)$. The Kantorovich formulation of Optimal Transport [1] considers the minimum transport cost over couplings of μ and ν .

Definition 1 (Kantorovich Formulation of optimal transport). Let μ, ν be measures on \mathcal{X} and d a metric on \mathcal{X} , we define the set of couplings of μ and ν to be $\Pi(\mu, \nu) := \{\pi \in \mathcal{P}(\mathcal{X}^2) : \pi(A \times \mathcal{X}) = \mu(A), \pi(\mathcal{X} \times B) = \nu(B)\}$. Then we define the Wasserstein p distance by:

$$W_p(\mu, \nu)^q = \inf_{\pi \in \Pi(\mu, \nu)} \left(\int_{\mathcal{X}^2} d(x, y)^p d\pi \right). \quad (1)$$

It is known that W_p is a metric on the space of (finite p 'th moment) measures on \mathcal{X} , see [2, Definition 6.4]. The Wasserstein distance is popular in machine learning circles, namely as a loss function [3]–[5] and utilising its Riemannian structure for Wasserstein Gradient Flows [6], [7]. One notable development connecting optimal transport and differential geometry came via the Benamou-Brenier formulation, which re-parametrised the minimisation in terms of time-dependent distribution and velocity field pairs (f_t, v_t) .

Proposition 1 (Benamou-Brenier Formulation). Given two distributions $f(0), f(1) \in \mathcal{P}(\mathbb{R}^d)$, we can then express

$$W_p(f(0), f(1)) = \inf_{(f_t, v_t)} \left(\int_0^1 \int ||v_t||^p df_t dt \right)^{\frac{1}{p}} \quad (2)$$

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where (f_t, v_t) are constrained by the transport equation - also known as the continuity equation:

$$\partial_t f_t + \nabla \cdot (f_t v_t) = 0 \quad (3)$$

where $\nabla \cdot$ is the divergence operator, (see [8]).

Definition 2 (Constant Speed Geodesics). Given a metric space (\mathcal{X}, d) , we say a path f_t is a *Constant Speed Geodesic* if and only if $d(f_s, f_t) = |s - t|d(f_0, f_1)$ and for a general path we define its *Speed* as $|\dot{f}|_d = \lim_{h \rightarrow 0} \frac{1}{h} d(f_{t+h}, f_t)$. Constant speed geodesics have constant speed, see [2, Remark 7.7].

The infimum in (2) is achieved by choosing f_t as a constant speed W_p geodesic and v_t satisfying $||v_t|| = |\dot{f}|_{W_p}$, (see [8]).

On \mathbb{R}^d , the constant speed W_p geodesics are the McCann displacement interpolations, see [9, Definition 1.1]. Though for discrete measures, say on $\{0, 1, \dots, n\} \subset \mathbb{R}$, the McCann interpolations will traverse \mathbb{R} , but not remain in the domain $\{0, 1, \dots, n\}$. This means to interpolate across discrete domains, considering them as embedded in a continuum will not suffice. This unfortunately sacrifices the classical Benamou-Brenier formula.

Work has already been done to amend this. Maas [10], gave a discrete transport equation and a new metric \mathcal{W} , distinct from W_2 , which minimised a kinetic energy functional and interplayed well with discrete gradient flows.

Beckmann [11] provided a (time independent) velocity field formulation of W_1 on both continuous and discrete domains which preceded Benamou and Brenier. A concise reference can be found in [12, Section 6.3].

Finally, Hillion and Johnson [13] provided conditions for a discrete Benamou-Brenier formulation on \mathbb{Z} , which we are building on. In this paper we offer our own discrete transport equation including triples (f, v, g) , and derive a Benamou-Brenier formulation for W_1 on trees (Lemma 2, Theorem 1). We then generalise this result to graphs (Lemma 3, Theorem 2) and classify the constant speed W_1 geodesics via the solutions to our formulation (Proposition 4).

II. NOTATION AND THE DISCRETE TRANSPORT EQUATION

Example 1. Consider the path of Binomial distributions $f(t) = \text{Bin}(n, p(t))$ on the set $\mathcal{V} = \{0, 1, \dots, n\}$ and p varies with time. We show the case $n = 5$ below:



By the product rule and some rudimentary combinatorics we can express the derivative as:

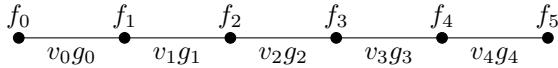
$$\begin{aligned}\partial_t f_x &= np' \text{Bin}_{x-1}(n-1, p) - np' \text{Bin}_x(n-1, p) \\ &= -\nabla_1(np' \text{Bin}_x(n-1, p))\end{aligned}$$

where $\nabla_1(h_x) := h_x - h_{x-1}$ is the finite difference operator.

This resembles (3), yet the distribution inside the spatial derivative is no longer f , in fact it is another distribution g , that has support $\{0, 1, \dots, n-1\}$. This means the discrete transport equation satisfied in this case is

$$\partial_t f + \nabla_1(vg) = 0$$

where $v(t) = np'$ and $g(t) = \text{Bin}(n-1, p)$. Our key insight is that \mathcal{V} can be considered as the vertices of a path graph \mathcal{G} , and that g and v exists on the edges of \mathcal{G} as follows:



and the discrete transport equation states that the rate of change at node x is the potential difference across that node. On a general graph, we do not have the canonical rightward direction of edges for mass to flow, so in some sense on a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ we must choose this orientation arbitrarily.

A. Matrices, Operators, Equations and Integrals

In this section, we will define our necessary objects. This includes a divergence operator, a discrete transport equation, and an energy functional, which we aim to minimise, as constrained by the discrete transport equation.

Definition 3 (Incidence Matrix and Arrow Shorthand). Given a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, we define the incidence matrix $\Omega = (\omega_{x,k})_{x \in \mathcal{V}, k \in \mathcal{E}}$, by

$$\omega_{x,k} = \begin{cases} 1 & : k \text{ is incoming to } x \\ -1 & : k \text{ is outgoing from } x \\ 0 & \text{otherwise.} \end{cases}$$

As shorthand for $\omega_{x,k} = 1$ and $\omega_{k,x} = -1$ we will write $x \rightarrow k$ and $k \rightarrow x$ respectively.

For example, we could orient \mathbb{Z} by directing edges away from 0, rather than left to right.

Definition 4 (Floor and Ceiling Notation). Given an edge $k \in \mathcal{E}$, we denote $\lceil k \rceil$ to be the node it is incoming to, and $\lfloor k \rfloor$ to be the node it is outgoing from.

Now, we can use the incidence matrix to define discrete derivative and divergence operators between functions on vertices and edges respectively.

Definition 5 (The Gradient and Divergence Operator). Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a graph with incidence matrix Ω . Then

- 1) For a function f defined on vertices \mathcal{V} , we define the *Gradient Operator* at edge $k \in \mathcal{E}$ to be:

$$(\nabla f)_k := (-\Omega^T \cdot f)_k = -\sum_{x \in \mathcal{V}} \omega_{x,k} f_x = f_{\lceil k \rceil} - f_{\lfloor k \rfloor},$$

i.e., the difference in function f along the edge k .

- 2) For a function g defined on the edges \mathcal{E} , we define the *Divergence Operator* at vertex $x \in \mathcal{V}$ to be:

$$(\nabla \cdot g)_x := -\Omega \cdot g = -\sum_{k \in \mathcal{E}} \omega_{x,k} g_k = \sum_{k: x \rightarrow k} g_k - \sum_{k: k \rightarrow x} g_k,$$

i.e., the difference in total flow out of and flow into x .

If we consider ∇_1 as instead defined on edges $(x, x-1)$ of \mathbb{Z} , it corresponds exactly to the $\nabla \cdot$ operator. The composition $\mathcal{L} := \Omega \Omega^T$ is the Laplacian.

B. The Discrete Transport Equation

We now build a framework to generalise Example 1. We start by building the transport equation as satisfied by a triple (f, v, g) , where we impose that v and g exist on edges.

Definition 6 (Discrete Transport Equation). Given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with incidence matrix Ω , we say the transport equation is satisfied if: for a path of distributions on vertices $f = f(t)_x$, a path of functions on edges $v = v(t)_k$ (called the velocity), and a path of distributions on edges $g = g(t)_k$, we have

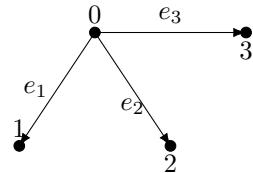
$$\partial_t f(t)_x + (\nabla \cdot v(t)g(t))_x \text{ for all } x \in \mathcal{V}, t \in [0, 1]. \quad (4)$$

This can be compactly expressed in terms of the incidence matrix Ω :

$$\partial_t f = \Omega \cdot (vg) \quad (5)$$

where the product vg is component-wise.

Example 2. Consider the following directed star graph S_3 :



and define f to be $f(t) = Z(1, s, s, s)$ for an arbitrary decreasing and positive $s(t)$ and partition function $Z(t) = \frac{1}{1+3s}$. This is the stationary distribution of a Markov jump process Q where $q_{x0}s(t) = q_{0x}$. Equation (4) states that

$$\begin{aligned}\partial_t f_0 &= -Z'(t) &= -v_{e_1}g_{e_1} - v_{e_2}g_{e_2} - v_{e_3}g_{e_3}, \\ \partial_t f_1 &= \frac{1}{3}Z'(t) &= v_{e_1}g_{e_1}, \\ \partial_t f_2 &= \frac{1}{3}Z'(t) &= v_{e_2}g_{e_2}, \\ \partial_t f_3 &= \frac{1}{3}Z'(t) &= v_{e_3}g_{e_3}.\end{aligned}$$

From here we have many choices for (v, g) . One of note is when v is invariant across edges, i.e., when we choose

$$v_{e_1} = v_{e_2} = v_{e_3} = Z'(t), \quad g_{e_1} = g_{e_2} = g_{e_3} = \frac{1}{3}.$$

We will return to this distribution and will motivate our choice of solution in Example 5.

We have our discrete transport equation, but a Benamou-Brenier formulation also requires an energy functional to minimise. In Proposition 1, we compute the expectation of v with respect to f . However since v exists on the edges with g , it is more natural to take the expectation over g . We keep the integral over time unchanged.

Definition 7 (Integral Formulation). Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a graph with incidence matrix Ω and suppose (f, v, g) satisfy (4). For $q \geq 1$ we define

$$\mathcal{I}_q(v, g) := \left(\int_0^1 \sum_{k \in \mathcal{E}} g_k(t) |v_k(t)|^q dt \right)^{\frac{1}{q}}. \quad (6)$$

Then for two distributions $f(0), f(1)$ on \mathcal{V} , we define

$$V_q(f(0), f(1)) := \inf_{f, v, g} \{ \mathcal{I}_q(v, g) : \partial_t f = \Omega \cdot (vg) \} \quad (7)$$

and so V_q is a measure of discrepancy between $f(0)$ and $f(1)$. This is a generalisation of a functional in [13, Definition 3.2], which is the work we are building on.

III. MAIN RESULTS

A. Benamou-Brenier on the Vertices of a Tree

The Wasserstein-1 distance on \mathbb{Z} has a closed form expression, see [14, Lemma 8.2]. Slightly lesser known is that a generalised expression for the tree exists too – thanks to Evans, [15] – which remarkably corresponds to a metric from Microbiology called the UniFrac metric, see [16]. Evans defines W_1 in terms of cuts, but for our purposes, we will formulate it in terms of tails. Let \mathcal{G} be a tree, and choose an arbitrary root node $r \in \mathcal{V}$ and define our incidence matrix by directing arrows away from r . This allows us to define tails.

Definition 8 (Tails of Distributions). We define the tail past $x \in \mathcal{V}$ to be

$$U(x) = \{y \in \mathcal{V} : \exists k_1, \dots, k_n (x \rightarrow k_1 \rightarrow \dots \rightarrow k_n \rightarrow y)\}$$

and then $F_x = \sum_{y \in U(x)} \mathbb{I}(y \in U(x)) f_y$ is called the *tail distribution of f past x* .

$U(x)$ and F_x generalise the set $\{x, x+1, x+2, \dots\}$ for \mathbb{Z} and the tail distribution on \mathbb{Z} respectively. Then we have the following result.

Proposition 2 (Wasserstein-1 on a Tree [15]). Given a rooted tree \mathcal{G} , for two distributions $f(0)$ and $f(1)$ on \mathcal{V} we have that

$$W_1(f(0), f(1)) = \sum_{x \in \mathcal{V}} |F(1)_x - F(0)_x|. \quad (8)$$

It is worth noting that we have other special cases of W_1 . For cyclic graphs, we have another closed form expression which utilises cuts, see [17] and for a general graph, W_1 can

be expressed as the minimum transport cost across possible spanning trees of \mathcal{G} , see [18].

Lemma 1 (Tail Variant of the Transport Equation). Let \mathcal{G} be a tree with root node r and incidence matrix Ω , if we denote the tail of f by $F(t)_x := \sum_y \mathbb{I}(y \in U(x)) f(t)_y$, we can invert (4) via the tail distributions:

$$\partial_t F(t)_{\lceil k \rceil} = v(t)_k g(t)_k, \quad (9)$$

and g can be derived exactly from f and v .

Proof. We drop the dependence on t for now, and consider:

$$\begin{aligned} \partial_t F_{\lceil k \rceil} &= \sum_{y \in \mathcal{V}} \mathbb{I}(y \in U(\lceil k \rceil)) \partial_t f_y \\ &= \sum_{y \in \mathcal{V}} \mathbb{I}(y \in U(\lceil k \rceil)) \sum_{j \in \mathcal{E}} \omega_{y,j} v_j g_j \\ &= \sum_{j \in \mathcal{E}} v_j g_j \sum_{y \in \mathcal{V}} \omega_{y,j} \mathbb{I}(y \in U(\lceil k \rceil)) \\ &= \sum_{j \in \mathcal{E}} v_j g_j (\nabla \mathbb{I}(y \in U(\lceil k \rceil)))_j \\ &= \sum_{j \in \mathcal{E}} v_j g_j \mathbb{I}(j = k) \\ &= v_k g_k. \end{aligned}$$

Then g can be derived from f and v by rearranging (9). \square

While we have inverted (4), we still have a family of possible (v, g) which satisfy (9), below we discuss the most important case for our purposes.

Lemma 2 (Constant Speed Solutions). Given a path f , we define the *Constant Speed Solution* to be

$$v_k = \text{sign}(\partial_t F_{\lceil k \rceil}) |v|, \quad g_k = |\partial_t F_{\lceil k \rceil}| / |v| \quad (10)$$

where $|v| = \sum_{x \in \mathcal{V}} |\partial_t F(t)_x|$. For this we have $|v| = |\dot{f}|_{W_1}$, and if f is a constant speed geodesic, we additionally have that $\mathcal{I}_2(v, g) = |v| = W_1(f(0), f(1))$.

Proof. See Appendix A. \square

Theorem 1 (Benamou-Brenier across a tree). Let \mathcal{G} be a rooted tree, then we have

$$W_1(f(0), f(1)) = \inf_{f, g, v} \{ \mathcal{I}_2(v, g) : \partial_t = \Omega \cdot (vg) \}. \quad (11)$$

for all $f(0)$ and $f(1)$ on \mathcal{V} . The minimum is achieved by a constant speed geodesic f , and the velocity v satisfies $|v(t)_k| = |\dot{f}|_{W_1}$, analogous to the continuous case.

Proof. An immediate consequence of (8) and (9) is we are given an integral formulation of W_1 . Remarkably, if (f, v, g) is any triple which satisfies (4), then we can write

$$\begin{aligned} W_1(f(0), f(1)) &= \sum_{x \in \mathcal{V}} |F(1)_x - F(0)_x| \\ &= \sum_{x \in \mathcal{V}} \left| \int_0^1 \partial_t F(t)_x dt \right| \\ &= \sum_{k \in \mathcal{E}} \left| \int_0^1 g(t)_k v(t)_k dt \right| \end{aligned}$$

which transforms a sum over tails to a sum over edges. Squaring both sides and applying both Jensen's and the Cauchy Schwarz inequalities bounds W_1 above by V_2 .

$$\begin{aligned} W_1(f(0), f(1))^2 &= \left(\sum_{k \in \mathcal{E}} \left| \int_0^1 g(t)_k v(t)_k dt \right| \right)^2 \\ &\leq \left(\int_0^1 \sum_{k \in \mathcal{E}} |g(t)_k v(t)_k| dt \right)^2 \\ &\leq \int_0^1 \left(\sum_{k \in \mathcal{E}} |g(t)_k v(t)_k| \right)^2 dt \\ &\leq \int_0^1 \sum_{k \in \mathcal{E}} g(t)_k |v(t)_k|^2 dt = \mathcal{I}_2(v, g)^2 \end{aligned}$$

So, we have that $V_2 \geq W_1$ too. However, Lemma 2, says that a constant speed solution achieves W_1 , so choosing an arbitrary constant speed geodesic as in Definition 2 - see Appendix B for an explicit example - we have that $V_2(f(0), f(1)) = W_1(f(0), f(1))$ and we are done. \square

In fact, the proofs for Lemma 2 and Theorem 1 work for $q \geq 1$ too, so we have a more general result that $V_q = W_1$, (see Appendix. C) and we can choose q arbitrarily.

Example 3. Consider Example 1 when $p(t) = (1-t)p + tq$ for $p > q > 0$. We know that $v(t) = n(q-p)$ and $g(t) = \text{Bin}(n-1, p(t))$ satisfy (4). We also have that $\mathcal{I}_2(v, g) = n(q-p) = W_1(f(0), f(1))$, so the original choice of (f, v, g) is minimizing. This solution also contains a constant speed geodesic in the form of f .

Example 4. Let $f(t) = \text{Poi}((1-t)\lambda + t\mu)$, then $v(t) = \mu - \lambda$ and $g(t) = \text{Poi}((1-t)\lambda + t\mu)$ also satisfy (4) and $\mathcal{I}_2(v, g) = \lambda - \mu = W_1(f(0), f(1))$. Again f is a constant speed geodesic.

Example 5. Consider Example 2. When $s(t) = \frac{-1}{3}(1 + \frac{1}{at+b})$ for $a, b < -1$, we have that s is both decreasing and positive. We can also show that $Z''(t) = 0$. So by choosing the edge invariant solution we know $Z'(t) = v_{01} = v_{02} = v_{03}$ are also constant in time. Plugging this into \mathcal{I}_2 we have

$$\mathcal{I}_2(v, g) = \int_0^1 Z'(t) dt = Z(1) - Z(1) = W_1(f(0), f(1)).$$

For this choice of $s(t)$, we have that $f(t) = (1-t)f(0) + tf(1)$ and by Appendix B this is a constant speed geodesic.

We cannot apply the same argument to the graph case as in the tree, to work toward the graph, we will build a *Reduced Formulation* of V_q by studying the solutions to (4) in more detail.

B. The Reduced Formulation on a Graph

In the continuous formulation, so long as smoothness assumptions were made, switching from f_t to v_t and vice versa was a matter of solving a first-order PDE, see [19, Chapter 16.1] for details. However, in our case, we can solve this more directly - although different methods are required for each direction.

Remark 1. Given f , solving (5) for (v, g) involves inverting Ω . Fortunately there is a plethora of work on solving these systems, see [20, Section 2]. For an incidence matrix Ω , we have $\text{Im}(\Omega) = \{x : \sum_j x_j = 0\}$ and $\text{rank}(\Omega) = |\mathcal{V}| - 1$, see [20, Lemma 2.4]. We know $\partial_t f \in \text{Im}(\Omega)$ for all t , so we can always solve for the vector vg . Although, this system is not full rank. Removing an arbitrary row r from f and Ω gives

$$\partial_t \tilde{f} = \tilde{\Omega} \cdot (vg)$$

which is full rank. Then for an arbitrary right inverse P (such that $\tilde{\Omega}P = I$) we can express the general solution as

$$vg = P \cdot \partial_t \tilde{f} + \epsilon$$

for some $\epsilon \in \ker(\Omega)$. One can find a right inverse by choosing a spanning tree \mathcal{T} and considering its *path matrix* $P_{\mathcal{T}}$, the right inverse then has block structure including $P_{\mathcal{T}}$. This additionally characterises $\ker(\Omega)$ as the cycle space of Ω , see [20, Theorem 2.13]. In the case that \mathcal{G} is a tree, $\tilde{\Omega}$ is invertible, and $\tilde{\Omega}^{-1}$ is defined by (9). For each valid (P, ϵ) we have a family of solutions for (v, g) .

Remark 2. Suppose we instead have a pair (v, g) on the edges of a graph, we can create a path f on the vertices as follows:

$$f(t)_x = \int_0^t \sum_{k \in \mathcal{E}} \omega_{x,k} v(\tau)_k g(\tau)_k d\tau + f(0)_x \quad (12)$$

and for shorthand we denote $f = \int \Omega \cdot (vg)$. Conversely, for any path $f(t)$ on the vertices, no matter which (v, g) pair we choose as a solution to (4) we can reconstruct f by using (12).

The lack of a unique inverse prevents us from obtaining g in terms of f and v or v in terms of f and g . However we can use Remark 2, to limit our search for pairs (v, g) living on the edges of \mathcal{G} .

Proposition 3 (Reduced Formulation). We have that

$$V_q(f(0), f(1)) = \inf_{v, g} \left\{ \mathcal{I}_q(v, g) : f(1) - f(0) = \Omega \int_0^1 gv dt \right\}$$

Proof. By Remark 2, we have a surjection $(v, g) \mapsto f$ such that $\partial_t f = \Omega \cdot (vg)$, so searching over triples (f, v, g) accounts to searching over (v, g) and inducing a path f via Equation (12). However we require the constructed f to truly interpolate between $f(0)$ and $f(1)$, which can only happen if

$$\int_0^1 \sum_{k \in \mathcal{E}} \omega_{x,k} g(t)_k v(t)_k dt = f(1) - f(0). \quad (13)$$

As shorthand we denote $\Omega \cdot \int_0^1 gv dt = f(1) - f(0)$. \square

This formulation is connected to the Beckmann formulation [11], albeit with time-dependent parameters.

Remark 3. We have a new condition given by (13). So we should also investigate the structure of solutions, fortunately we can inherit most of the machinery from Remark 1, as we are still inverting an incidence matrix. We have that (v, g) must satisfy

$$\int_0^1 vg dt = P \cdot [\tilde{f}(1) - \tilde{f}(0)] + \epsilon \quad (14)$$

for some P such that $\Omega \cdot P = I$ and $\epsilon \in \ker \Omega$.

C. Benamou-Brenier on the Vertices of a graph

The multiple constant speed solutions explains why we cannot extend the argument of Section III-A to a graph. In fact not all constant speed solutions will minimize V_q , never mind integrate to W_1 . However we can demonstrate that these solutions minimize \mathcal{I}_q for a given P and ϵ .

Lemma 3 (Generalised Constant Speed Solutions). Given a graph \mathcal{G} and (P, ϵ) a valid choice for inverting Ω , define the *Constant Speed Solution* associated to (P, ϵ) to be

$$v_k = \text{sign}(P \cdot \tilde{f} + \epsilon)_k |v|, \quad g_k = |P \cdot \tilde{f} + \epsilon|_k / |v| \quad (15)$$

where $|v| = \sum_{k \in \mathcal{V}} |P \cdot \tilde{f} + \epsilon|_k$. Then the constant speed solution minimizes $\mathcal{I}_q(v, g)$ over the pairs (v, g) associated to (P, ϵ) , i.e pairs which satisfy (14).

Proof. See Appendix D. \square

On a tree, we have one inverse (up to choice of root node) and Lemma 3 is equivalent to the constant speed solution minimising $\mathcal{I}_q(v, g)$, which is implied by Theorem 1.

We now present the main result of the paper: showing that the Benamou-Brenier formula holds for $q \geq 1$ on a general connected graph.

Theorem 2 (Benamou-Brenier across a Graph). For a connected graph \mathcal{G} , for any $q \geq 1$, we can express the Wasserstein-1 distance between $f(0)$ and $f(1)$ by

$$\inf_{f, v, g} \left\{ \left(\int_0^1 \sum_{k \in \mathcal{E}} g(t)_k |v(t)_k|^q dt \right)^{\frac{1}{q}} : \partial_t f = \Omega \cdot (vg) \right\} \quad (16)$$

where Ω is an arbitrary incidence matrix of \mathcal{G} , and the infimum is achieved for at least one triple (f, v, g) .

Proof. See Appendix E. \square

Remark 4 (Wasserstein Tree Distance). The proof of Theorem 2 is independent of the proof for the tree, meaning that the W_1 distance on a tree can be derived from Theorems 1 and 2.

The following proposition demonstrates our motivation for considering time dependent pairs (v, g) , instead of fixed flows along edges, in that they induce a family of constant speed W_1 geodesics.

Proposition 4 (Geodesics). Given a pair (v, g) which achieves W_1 , the induced path f is a constant speed W_1 geodesic. Conversely, if f is a constant speed geodesic, then there exists (v, g) which achieves W_1 and induces f .

Proof. Suppose that (v, g) minimises \mathcal{I}_1 . If it has constant speed, proceed, else substitute it for a constant speed solution as in Lemma 2. Then we define the path $f(t) = \int \Omega(vg)d\tau$ for $t \in [0, 1]$. For an arbitrary subinterval $[s, t]$, the triple (f, v, g) restricted to $[s, t]$ is still a solution to (5). What is unclear, is whether it is a minimising solution too. Suppose there exists \tilde{v}, \tilde{g} such that

$$\int_s^t \sum_{k \in \mathcal{E}} \tilde{g}(\tau)_k |\tilde{v}(\tau)_k| d\tau < \int_s^t \sum_{k \in \mathcal{E}} g(\tau)_k |v(\tau)_k| d\tau.$$

Define a piecewise new pair (\hat{v}, \hat{g}) defined on $[0, 1]$ by

$$(\hat{v}, \hat{g}) = \begin{cases} (\tilde{v}, \tilde{g}) & : \tau \in [s, t] \\ (v, g) & : \tau \notin [s, t]. \end{cases}$$

But then by linearity of the integral we will have $\mathcal{I}_1(\tilde{v}, \tilde{g}) < \mathcal{I}_1(v, g)$ and hence (v, g) is not a minimiser. So (v, g) is a minimising solution between $[s, t]$ too and we have

$$\begin{aligned} W_1(f(s), f(t)) &= \int_s^t |v| d\tau \\ &= (t-s) \int_0^1 |v| d\tau = |t-s| W_1(f(0), f(1)) \end{aligned}$$

and so f is a constant speed geodesic.

Now suppose f is a constant speed geodesic, we will use the result that the W_1 distance on a graph \mathcal{G} is equal to W_1 across one of the spanning trees of \mathcal{G} , which we call \mathcal{T} . Then, we choose (v, g) as the constant speed solution as in Lemma 2. This pair achieves W_1 on \mathcal{T} and hence on \mathcal{G} . \square

Corollary 1 (Convex Interpolations are W_1 Geodesics). Let $f(0), f(1)$ be two distributions on the vertices of a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, then $f(t) = (1-t)f(0) + tf(1)$ is a constant speed W_1 geodesic.

Proof. Let J be a minimising flow in the Beckmann formulation, then we choose, $v_k g_k = J_k$. This achieves W_1 and then $f(t) = \int_0^t \Omega \cdot J d\tau = t(f(1) - f(0)) + f(0)$ is a constant speed W_1 geodesic. \square

IV. CONCLUSION

We have extended the work of Hillion and Johnson (see [13, Lemma 3.6]) to demonstrate that the discrete Benamou-Brenier formulation of W_1 holds in generality on \mathbb{Z} , on trees, and eventually on graphs. The tree case lends itself particularly well, with an exact form for the minimizing triples in terms of tail distributions of a constant speed geodesics.

While the minimal Beckmann flow provides us with a convex interpolation (see Corollary 1), we see that on \mathbb{Z} and even cycles we have minimizing triples (f, v, g) with more exotic geodesics (see Examples 3,4 and Appendix F). We formalise this characterisation of constant speed W_1 geodesics in Proposition 4.

APPENDIX

A. Proof of Lemma 2 for $q \geq 1$

Proof. Let us compute $|\dot{f}|_{W_1}$ directly, we have that

$$\begin{aligned} |\dot{f}|_{W_1} &= \lim_{h \rightarrow 0} \frac{W_1(f(t+h), f(t))}{h} \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \sum_{x \in \mathcal{V}} |F(t+h)_x - F(t)_x| \\ &= \sum_{x \in \mathcal{V}} \left| \lim_{h \rightarrow 0} \frac{F(t+h)_x - F(t)_x}{h} \right| \\ &= \sum_{x \in \mathcal{V}} |\partial_t F(t)_x| = |v|(t). \end{aligned}$$

Now assume that f is a constant speed geodesic, we know from Definition 2 that

$$W_1(f(t+h), f(t)) = |h| W_1(f(0), f(1)),$$

re-arranging and taking limits we have

$$|v| = |\dot{f}|_{W_1} = \lim_{h \rightarrow 0} \frac{W_1(f(t+h), f(t))}{|h|} = W_1(f(0), f(1)).$$

So overall we have

$$\begin{aligned} \mathcal{I}_q(v, g)^q &= \int_0^1 \sum_{k \in \mathcal{E}} g(t)_k v(t)_k^q dt \\ &= \int_0^1 \sum_{k \in \mathcal{E}} g(t)_k |v|^q dt \\ &= \int_0^1 |v|^q dt \\ &= |v|^q = W_1(f(0), f(1))^q \end{aligned}$$

and so $\mathcal{I}_q(v, g) = W_1(f(0), f(1))$. \square

B. Proof that Convex Interpolation is a Geodesic on a Tree

Proof. Consider a convex interpolation $f(t) = (1-t)f(0) + tf(1)$, then the tail distribution is similarly convex $F(t) = (1-t)F(0) + tF(1)$. Then we directly compute:

$$\begin{aligned} W_1(f(s), f(t)) &= \sum_{x \in \mathcal{V}} |F(s)_x - F(t)_x| \\ &= \sum_{x \in \mathcal{V}} |(1-s)F(0)_x + sF(1)_x \\ &\quad - (1-t)F(0)_x - tF(1)_x| \\ &= \sum_{x \in \mathcal{V}} |(t-s)(F(1)_x - F(0)_x)| \\ &= |t-s| \sum_{x \in \mathcal{V}} |F(1)_x - F(0)_x| \\ &= |s-t| W_1(f(0), f(1)). \end{aligned}$$

So f is a constant speed geodesic. \square

C. Proof of Theorem 1 for $q \geq 1$

Proof. An immediate consequence of (8) and (9) is we are given an integral formulation of W_1 . Remarkably, if (f, v, g) is any triple which satisfies (4), then we can write

$$\begin{aligned} W_1(f(0), f(1)) &= \sum_{x \in \mathcal{V}} |F(1)_x - F(0)_x| \\ &= \sum_{x \in \mathcal{V}} \left| \int_0^1 \partial_t F(t)_x dt \right| \\ &= \sum_{k \in \mathcal{E}} \left| \int_0^1 g(t)_k v(t)_k dt \right| \end{aligned}$$

which transforms a sum over tails to a sum over edges. Although this goes further, by applying both Jensen's and the Cauchy Schwarz inequalities, we can bound W_1 above by V_q .

$$\begin{aligned} W_1(f(0), f(1))^q &= \left(\sum_{k \in \mathcal{E}} \left| \int_0^1 g(t)_k v(t)_k dt \right| \right)^q \\ &\leq \left(\int_0^1 \sum_{k \in \mathcal{E}} |g(t)_k v(t)_k| dt \right)^q \\ &\leq \int_0^1 \left(\sum_{k \in \mathcal{E}} |g(t)_k v(t)_k| \right)^q dt \\ &\leq \int_0^1 \sum_{k \in \mathcal{E}} g(t)_k |v(t)_k|^q dt = \mathcal{I}_q(v, g)^q \end{aligned}$$

So we have that $V_q \geq W_1$ too. However, Lemma 2, says that a constant speed solution achieves W_1 , so we in fact have that $V_q(f(0), f(1)) = W_1(f(0), f(1))$ and we are done. \square

D. Proof of Lemma 3

Proof. We write $\int_0^1 vgdt = P \cdot (f(1) - f(0)) + \epsilon$ for inverse P and $\epsilon \in \ker \Omega$. Let (\tilde{v}, \tilde{g}) be the constant speed solution, i.e., $|\tilde{v}(t)_j| = \sum_k |P \cdot (f(1) - f(0)) + \epsilon|$, then for any other solution associated to (P, ϵ) , say (v, g) , we have

$$\begin{aligned} \mathcal{I}_q(v, g)^q &= \int_0^1 \sum_k g(t)_k |v(t)_k|^q dt \\ &\geq \left(\int_0^1 \sum_k |g(t)_k v(t)_k| dt \right)^q \\ &\geq \left(\sum_k \left| \int_0^1 g(t)_k v(t)_k dt \right| \right)^q \\ &= \left(\sum_k |P \cdot (f(1) - f(0)) + \epsilon| \right)^q \\ &= \int_0^1 |\tilde{v}|^q dt \\ &= \int_0^1 \sum_{k \in \mathcal{E}} \tilde{g}(t)_k |\tilde{v}(t)_k|^q dt = \mathcal{I}_q(\tilde{v}, \tilde{g})^q \end{aligned}$$

\square

E. Proof of Theorem 2

Proof. We first use the reduced form for V_q :

$$V_q(f(0), f(1)) = \inf_{v,g} \left\{ \mathcal{I}_q(v, g) : f(1) - f(0) = \Omega \int_0^1 gv dt \right\}$$

We can express the Beckmann formulation of the W_1 distance as follows:

$$W_1(f(0), f(1)) = \inf_J \left\{ \sum_{k \in \mathcal{E}} |J_k| : \Omega \cdot J = f(1) - f(0) \right\}$$

We begin by showing that $V_q \geq W_1$, let (v, g) satisfy

$$\Omega \cdot \int_0^1 gv dt = f(1) - f(0).$$

We see that identifying $J := \int_0^1 gv dt$ gives a valid solution to Beckmann's formulation. Then we have that

$$\begin{aligned} \mathcal{I}^q(v, g)^q &= \int_0^1 \sum_k g(t)_k |v(t)_k|^q dt \\ &\geq \int_0^1 \left(\sum_k |g(t)_k v(t)_k| \right)^q dt \\ &\geq \left(\int_0^1 \sum_k |g(t)_k v(t)_k| dt \right)^q \\ &\geq \left(\sum_k \int_0^1 |g(t)_k v(t)_k| dt \right)^q \\ &\geq \left(\sum_k \left| \int_0^1 g(t)_k v(t)_k dt \right| \right)^q \\ &= \left(\sum_k |J_k| \right)^q \\ &\geq W_1(f(0), f(1))^q \end{aligned}$$

So we have additionally that $V_q \geq W_1$. Conversely, choose J a minimising solution (achieves W_1) to the Beckmann formulation, then we can choose $|v| = \sum_k |J_k|$, $v(t)_k = \text{sign}(J_k)|v|$ and $g(t)_k = |J_k|/|v|$, which satisfies $g(t)_k v(t)_k = J_k$. Additionally this pair (v, g) is constant in time, so we have that

$$\Omega \cdot \int_0^1 gv dt = \Omega \cdot (gv) = \Omega \cdot J = f(1) - f(0).$$

So (v, g) satisfy the condition for V_q , then we have that

$$\begin{aligned} \left(\sum_k |J_k| \right)^q &= |v|^q \\ &= \sum_k g(t)_k |v(t)_k|^q \\ &= \sum_k g(t)_k |v(t)_k|^q \\ &= \int_0^1 \sum_k g(t)_k |v(t)_k|^q dt \\ &\geq V_q(f(0), f(1))^q \end{aligned}$$

So we additionally have $W_1 \geq V_q$, so overall we have that for any $f(0)$ and $f(1)$, we have

$$W_1(f(0), f(1)) = V_q(f(0), f(1)).$$

□

F. Supplementary Results

The following results are true by virtue of $V_q = W_1$, although contain useful insights nevertheless, including a proof that Wasserstein-1 is bounded below by the total variation.

Lemma 4. $V_q(f(0), f(1)) \geq \text{TV}(f(0), f(1))$ for all $q \geq 1$, where TV is the total variational distance.

Proof. Consider the reduced form of V_q , and let (v, g) satisfy

$$\Omega \cdot \int_0^1 vg dt = f(1) - f(0).$$

Writing this out explicitly we have

$$\begin{aligned} |f(1)_x - f(0)_x| &= \left| \int_0^1 \sum_{k \rightarrow x} g(t)_k v(t)_k - \sum_{x \rightarrow k} g(t)_k v(t)_k dt \right| \\ &\leq \int_0^1 \left| \sum_{k \rightarrow x} g(t)_k v(t)_k - \sum_{x \rightarrow k} g(t)_k v(t)_k \right| dt \\ &\leq \int_0^1 \sum_{k \rightarrow x} |g(t)_k v(t)_k| + \sum_{x \rightarrow k} |g(t)_k v(t)_k| dt. \end{aligned}$$

But considering the identity

$$\sum_x \sum_{k: k \rightarrow x} h_k + \sum_x \sum_{k: x \rightarrow k} h_k = 2 \sum_k h_k$$

we have that

$$\sum_x |f(1)_x - f(0)_x| \leq 2 \int_0^1 \sum_k |g(t)_k v(t)_k| dt.$$

Finally we have that

$$\begin{aligned} \mathcal{I}_q(v, g)^q &\geq \int_0^1 \sum_k g(t)_k |v(t)_k|^q dt \\ &\geq \int_0^1 \left(\sum_k |g(t)_k v(t)_k| \right)^q dt \\ &\geq \left(\int_0^1 \sum_k |g(t)_k v(t)_k| \right)^q \\ &\geq \left(\frac{1}{2} \sum_x |f(1)_x - f(0)_x| \right)^q = \text{TV}(f(0), f(1))^q. \end{aligned}$$

So $V_q \geq \text{TV}$ too.

□

Proposition 5. V_q defines a metric on $\mathcal{P}(\mathcal{V})$.

Proof. We begin with positive definiteness, we know $\mathcal{I}_q(v, g) \geq 0$ for all (v, g) , so $V_q \geq 0$. Additionally if $V_q(f(0), f(1)) = 0$, then $\text{TV}(f(0), f(1)) = 0$ too, so

$f(0) = f(1)$ since the total variation is a metric. Now we prove symmetry. For any pair (v, g) which satisfies

$$\Omega \cdot \int_0^1 gv dt = f(1) - f(0)$$

we can build a pair (\tilde{g}, \tilde{v}) by $\tilde{g}(t) = g(1-t)$ and $\tilde{v}(t) = -v(1-t)$ which satisfies

$$\begin{aligned} \Omega \cdot \int_0^1 \tilde{g}\tilde{v} dt &= -\Omega \cdot \int_0^1 g(1-t)v(1-t) dt \\ &= -\Omega \cdot \int_0^1 g(t)v(t) dt \\ &= f(0) - f(1). \end{aligned}$$

So (\tilde{g}, \tilde{v}) is valid for $V_q(f(1), f(0))$. Similarly we can see that $\mathcal{I}_q(\tilde{v}, \tilde{g}) = \mathcal{I}_q(v, g)$ too. If we consider a sequence $(g^{(n)}, v^{(n)})_n$ such that $\lim_{n \rightarrow \infty} \mathcal{I}_q(v^{(n)}, g^{(n)}) = V_q(f(0), f(1))$, then we induce a sequence $(\tilde{v}^{(n)}, \tilde{g}^{(n)})$ too, then

$$\begin{aligned} V_q(f(0), f(1)) &= \lim_{n \rightarrow \infty} \mathcal{I}_q(v^{(n)}, g^{(n)}) \\ &= \lim_{n \rightarrow \infty} \mathcal{I}_q(\tilde{v}^{(n)}, \tilde{g}^{(n)}) \\ &\geq V_q(f(1), f(0)). \end{aligned}$$

We can perform this process in reverse too, so $V_q(f(0), f(1)) = V_q(f(1), f(0))$. Finally we tackle the triangle inequality. We consider $f(0), f^*$ and $f(1)$, then let (v, g) be a pair between $f(0)$ and f^* and (\tilde{v}, \tilde{g}) be a pair between f^* and $f(1)$, then for some $\rho \in [0, 1]$ we define a piecewise solution

$$\hat{v}(t), \hat{g}(t) = \begin{cases} \frac{1}{\rho}v\left(\frac{t}{\rho}\right), g\left(\frac{t}{\rho}\right) & : t \in [0, \rho] \\ \frac{1}{1-\rho}\tilde{v}\left(\frac{t-\rho}{1-\rho}\right), \tilde{g}\left(\frac{t-\rho}{1-\rho}\right) & : t \in [\rho, 1] \end{cases}$$

It can be shown that

$$\mathcal{I}_q(\hat{v}, \hat{g})^q = \frac{1}{\rho}\mathcal{I}_q(v, g)^q + \frac{1}{1-\rho}\mathcal{I}_q(\tilde{v}, \tilde{g})^q$$

and we choose ρ such that

$$\mathcal{I}_q(\hat{v}, \hat{g})^q = (\mathcal{I}_q(v, g) + \mathcal{I}_q(\tilde{v}, \tilde{g}))^q$$

and hence

$$\mathcal{I}_q(\hat{v}, \hat{g}) = \mathcal{I}_q(v, g) + \mathcal{I}_q(\tilde{v}, \tilde{g}).$$

Then if we let $(g^{(n)}, v^{(n)})_n$ and $(\tilde{g}^{(n)}, \tilde{v}^{(n)})_n$ be sequences such that $\mathcal{I}_q(g^{(n)}, v^{(n)}) \rightarrow V_q(f(0), f^*)$ and $\mathcal{I}_q(\tilde{g}^{(n)}, \tilde{v}^{(n)}) \rightarrow V_q(f^*, f(1))$ respectively, then

$$\begin{aligned} V_q(f(0), f(1)) &\leq \lim_{n \rightarrow \infty} \mathcal{I}_q(\hat{v}^{(n)}, \hat{g}^{(n)}) \\ &= V_q(f(0), f^*) + V_q(f^*, f(1)) \end{aligned}$$

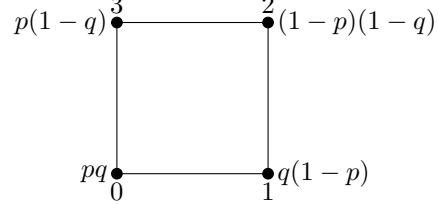
and we have the triangle inequality. Finally we motivate why we can choose ρ in such a way. We are essentially choosing ρ such that

$$\frac{1}{\rho}a^q + \frac{1}{1-\rho}b^q = (a+b)^q.$$

This is a quadratic in ρ which has valid solutions in $[0, 1]$. \square

The following is a worked example for finding valid minimizing solutions on a 4-cycle.

Example 6. Consider the following distribution f on a square generated by two probabilities p and q , we consider the Wasserstein distance between when $p = p_0, q = q_0$ and $p = p_1, q = q_1$ respectively.



Since these are product measures, we can show that $W_1(f(0), f(1)) = |p_1 - p_0| + |q_1 - q_0|$. We can express the transport equation as:

$$\begin{aligned} \partial_t f(t)_0 &= p'q + pq' &= -g_{01}v_{01} - g_{03}v_{03} \\ \partial_t f(t)_1 &= q'(1-p) - p'q &= g_{01}v_{01} - g_{12}v_{12} \\ \partial_t f(t)_2 &= -p'(1-q) - q'(1-p) &= g_{12}v_{12} + g_{32}v_{32} \\ \partial_t f(t)_3 &= p'(1-q) - pq' &= g_{03}v_{03} - g_{32}v_{32} \end{aligned}$$

Since we have one cycle, we know $\text{Nullity}(\Omega) = 1$, so we have one degree of freedom in solutions which are written as

$$\begin{aligned} g_{01}v_{01} &= -p'q + \epsilon \\ g_{03}v_{03} &= -pq' - \epsilon \\ g_{12}v_{12} &= q'(1-p) - \epsilon \\ g_{32}v_{32} &= p'(1-q) + \epsilon \end{aligned}$$

We choose a specific constant speed solution (v, g) by assigning $|v| = |p'| + |q'|$, then defining the velocity v by:

$$v_{01} = v_{32} = \text{sign}(p')|v|, \quad v_{03} = v_{12} = \text{sign}(q')|v|$$

and defining the edge distribution g by

$$\begin{aligned} |v|g_{01} &= |p'|q, & |v|g_{32} &= |p'|(1-q) \\ |v|g_{03} &= |q'|p, & |v|g_{12} &= |q'|(1-p) \end{aligned}$$

When p' and q' are constant, $|v|$ is additionally constant in time – as well as edge-wise. This constant speed solution achieves W_1 , so by Proposition 4, the induced path $f(t)$ is a geodesic. This corresponds to interpolating $p(t) = (1-t)p_0 + tp_1$ and $q(t) = (1-t)q_0 + tq_1$.

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