Optimal Transport on Graphs

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The Setting

Throughout, $\mathcal{G}$ is a **weighted graph** on nodes $\{1, \ldots, n\}$ with non-negative edge weights $\{q_{ij}\}_{i,j=1}^{n}$.

We require $\mathcal{G}$ to satisfy two key properties:

1. Symmetry: $q_{ij} = q_{ji}$ for all i, j.
2. Connectedness: For any two nodes i and j, there exists a path $i = k_0, k_1, \ldots, k_m = j$ such that $q_{k_\ell k_{\ell+1}} > 0$ for each step.

Any $p \in \mathcal{P}(\mathcal{G})$ can be written as $p = \sum_{i=1}^{n} p_i \delta_i$, where

1. $\forall i = 1, \ldots, n, p_i \geq 0$
2. $\sum_{i=1}^{n} p_i = 1$.

Throughout, we represent p via $[p_1, \ldots, p_n]$.

The Continuity Equation and the 2-Wasserstein Metric

For $\mu : [0,1] \to \mathcal{M}(\mathbb{R}^d)$, $v : [0,1] \times \mathbb{R}^d \to \mathbb{R}^d$, the continuity equation is

$$\partial_t \mu_t + \nabla \cdot (\mu_t v_t) = 0.$$

Benamou-Brenier Theorem

$$W_2^2(\mu_0, \mu_1) = \min \left\{ \int_0^1 \int_{\mathbb{R}^d} |v(t,x)|^2 d\mu_t \, dt : (\mu, v) \text{ solve continuity equation weakly} \right\}.$$

Intuition: Continuity equation ⇒ 2-Wasserstein distance. Is there a way to recover the CE in the graph setting?

The Graph Continuity Equation

Fix an interpolation function $\theta : [0, \infty) \times [0, \infty) \to [0, \infty)$.

Notation: $\check{p}v$

Let $p \in \mathcal{P}(\mathcal{G})$ and $v \in \mathbb{R}^{n \times n}$. We define $\check{p}v \in \mathbb{R}^{n \times n}$ by $(\check{p}v)_{ij} = \theta(p_i, p_j)v_{ij}$.

Notation: Graph Divergence

Let us define the graph divergence operator $\nabla_{\mathcal{G}} \cdot : \mathbb{R}^{n \times n} \to \mathbb{R}^n$. For $\psi \in \mathbb{R}^{n \times n}$,

$$(\nabla_{\mathcal{G}} \cdot \psi)_i := -\frac{1}{2} \sum_{j=1}^{n} (\psi_{ij} - \psi_{ji}) q_{ij}.$$

A pair $p : [0, 1] \to \mathcal{P}(\mathcal{G})$, $v : [0, 1] \to \mathbb{R}^{n \times n}$ satisfies the **graph continuity equation** if

$$\partial_t p_t + \nabla_{\mathcal{G}} \cdot (\check{p}_t v_t) = 0.$$

The Graph Wasserstein Space

Inspired by the Benamou-Brenier theorem, we define the **graph Wasserstein metric**

$$W_{\mathcal{G}}^2(p_0, p_1) = \inf \left\{ \int_0^1 \frac{1}{2} \sum_{i,j=1}^{n} |v_{ij,t}|^2 \, \theta(p_{i,t},\, p_{j,t}) \, q_{ij} \, dt : (p, v) \text{ solve graph CE weakly} \right\}.$$

There exists a constant $C_{\theta,\mathcal{G}}$ such that for all $p_0, p_1 \in \mathcal{P}(\mathcal{G})$,

$$\frac{1}{\sqrt{2}} |p_1 - p_0| \leq W_{\mathcal{G}}(p_0, p_1) \leq C_{\theta,\mathcal{G}} \sqrt{|p_1 - p_0|}.$$

Here, $|\cdot|$ is the Euclidean norm on $\mathcal{P}(\mathcal{G}) \subseteq \mathbb{R}^n$.

This implies that

1. $(\mathcal{P}(\mathcal{G}), W_{\mathcal{G}})$ has finite diameter.
2. The topology induced by $W_{\mathcal{G}}$ on $\mathcal{P}(\mathcal{G})$ is equivalent to the Euclidean topology on $\mathcal{P}(\mathcal{G}) \subseteq \mathbb{R}^n$, so $(\mathcal{P}(\mathcal{G}), W_{\mathcal{G}})$ is a complete metric space.

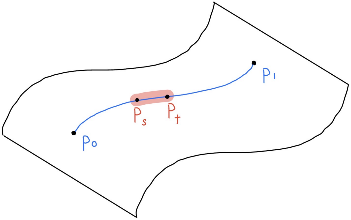
Geodesics

For any $p_0, p_1 \in \mathcal{P}(\mathcal{G})$, there exists a constant-speed geodesic $p \in AC(0,1;\mathcal{P}(\mathcal{G}))$ from p_0 to p_1. For any such geodesic, there exists a velocity field v such that (p, v) solves the graph continuity equation and

(a) $W_{\mathcal{G}}(p_t, p_s) = |t-s|\, W_{\mathcal{G}}(p_0, p_1)$ for all $s, t \in [0,1]$;

(b) $\|v_t\|_{\mathrm{Tan}_{p_t}\mathcal{P}(\mathcal{G})} = W_{\mathcal{G}}(p_0, p_1)$ for a.e. $t \in [0,1]$, where

$$\langle u, v\rangle_{\mathrm{Tan}_p\mathcal{P}(\mathcal{G})} := \frac{1}{2}\sum_{i,j=1}^{n} u_{ij}\, v_{ij}\, \theta(p_i, p_j)\, q_{ij}.$$



$$W_{\mathcal{G}}(p_t, p_s) = |t-s|\, W_{\mathcal{G}}(p_0, p_1)$$

Riemannian Structure on $(\mathcal{P}(\mathcal{G}))^\circ$

Note $(\mathcal{P}(\mathcal{G}))^\circ = \{p \in \mathcal{P}(\mathcal{G}) : p_i > 0 \text{ for all } 1 \leq i \leq n\}$.

The restriction of $W_\mathcal{G}$ to $(\mathcal{P}(\mathcal{G}))^\circ$ is a Riemannian distance, and $(\mathcal{P}(\mathcal{G}))^\circ$ is a smooth Riemannian manifold.

Caveat: $((\mathcal{P}(\mathcal{G}))^\circ, W_\mathcal{G})$ is **not geodesically complete**. For some pairs $p_0, p_1 \in \mathcal{P}(\mathcal{G}))^\circ$, the infimum in the $W_\mathcal{G}$ definition is not achieved by any curve remaining in the interior. The length-minimizing curve in the closure $\overline{\mathcal{P}(\mathcal{G})}$ hits the boundary $\partial\mathcal{P}(\mathcal{G})$ (where some $p_i = 0$), so no geodesic in $\mathcal{P}(\mathcal{G}))^\circ$ connects them.

Visualizing Our Manifold

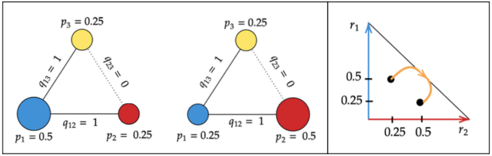
There is a bijection between $\mathcal{P}(\mathcal{G})$ and the simplex Δ^{n-1}:

1. Define $\mathbf{p} : \Delta^{n-1} \to \mathcal{P}(\mathcal{G})$ by $\mathbf{p}(r_1, \ldots, r_{n-1}) := \left[r_1,\ \ldots,\ r_{n-1},\ 1 - \sum_{i=1}^{n-1} r_i\right]$
2. Define $\mathbf{p}^{-1} : \mathcal{P}(\mathcal{G}) \to \Delta^{n-1}$ by $\mathbf{p}^{-1}[p_1, \ldots, p_n] := (p_1, \ldots, p_{n-1})$.

Since we have a metric on $\mathcal{P}(\mathcal{G})$ and a bijection from $\mathcal{P}(\mathcal{G})$ to Δ^{n-1}, we can induce a topology on the simplex:

$$d_{\Delta^{n-1}}(r, \tilde{r}) = W_{\mathcal{G}}(\mathbf{p}(r), \mathbf{p}(\tilde{r})).$$

With this intuition, we can see how the manifold is not complete:



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Interpolation Functions

Assumption 1.1 (Craig, García Trillos, Nikolić 2025)

$\theta : [0,\infty) \times [0,\infty) \to [0,\infty)$ satisfies:

- **(A1) Regularity:** θ is continuous on $[0,\infty) \times [0,\infty)$ and C^∞ on $(0,\infty) \times (0,\infty)$.
- **(A2) Symmetry:** $\theta(t,s) = \theta(s,t)$ for all $t, s \geq 0$.
- **(A3) Positivity:** $\theta > 0$ on $(0,\infty) \times (0,\infty)$.
- **(A4) Normalization:** $\theta(1,1) = 1$.
- **(A5) Monotonicity:** $\theta(r,t) \leq \theta(s,t)$ for $t \geq 0$ and $0 \leq r \leq s$.
- **(A6) Positive homogeneity:** $\theta(\lambda t, \lambda s) = \lambda\,\theta(t,s)$ for $\lambda > 0$, $t, s \geq 0$.
- **(A7) Concavity:** θ is concave.

Examples:

- Arithmetic mean: $\theta(s,t) = \dfrac{s+t}{2}$
- Geometric mean: $\theta(s,t) = \sqrt{st}$
- Logarithmic mean: $\theta(s,t) = \displaystyle\int_0^1 s^{1-\alpha} t^{\alpha}\, d\alpha$