Measure-valued spline curves: An optimal transport viewpoint

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(Literature Review by Manas Bhatnagar)

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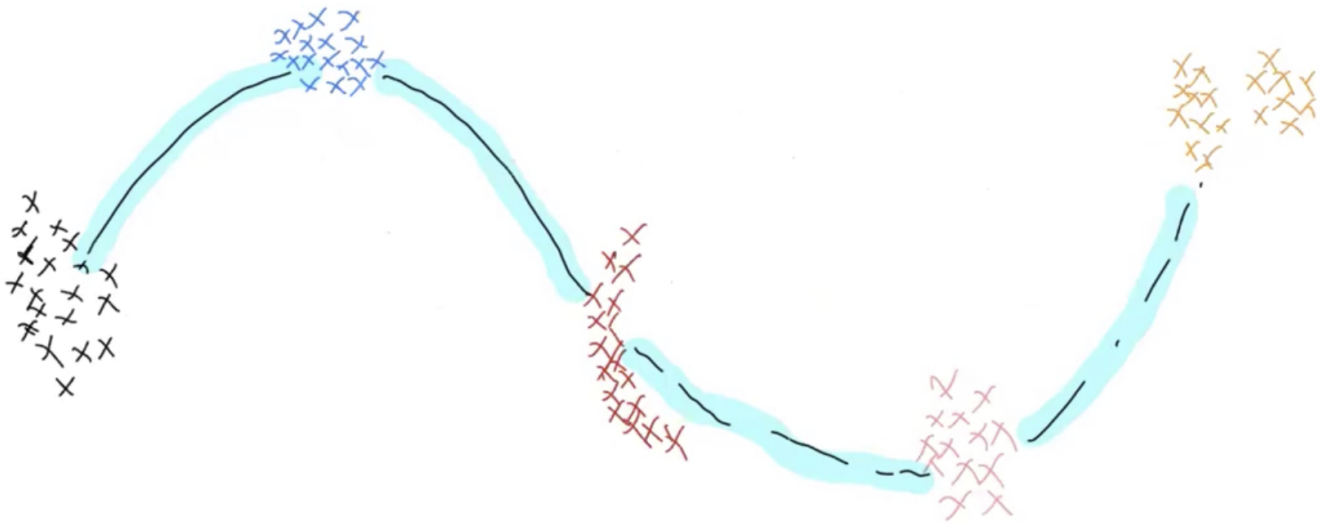
Introduction

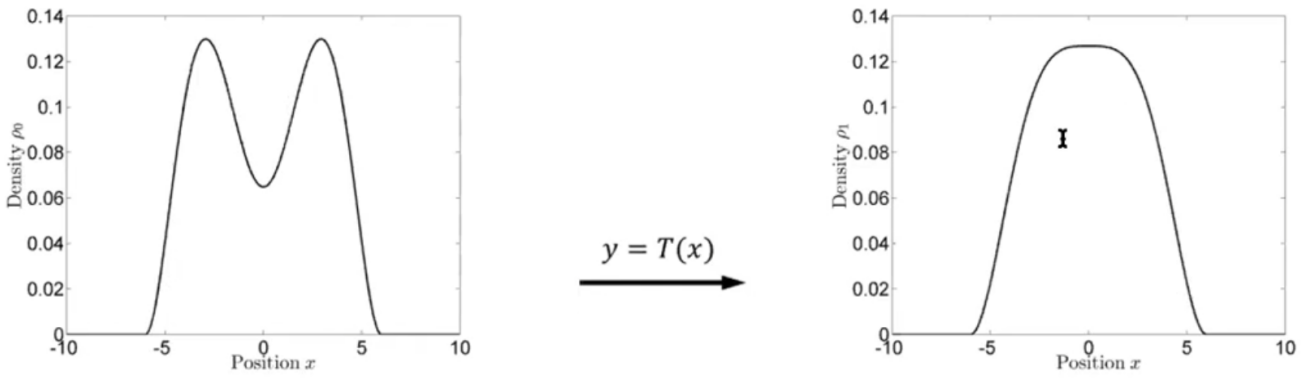
Motive

Smooth interpolation of distributions



Optimal Mass Transport

Move mass from distribution ρ_0 to ρ_1.



ρ_0 ρ_1

Monge's formulation:

$$\inf_{T_{\#}\rho_0=\rho_1} \int_{\mathbb{R}^d} c(x, T(x))\rho_0(x)\, dx.$$

- $c(x, y)$ is the cost function. Generally, $c(x, y) = |x - y|^2$.
- $T_{\#}\rho_0 := \rho_0 \circ T^{-1}$ is the pushforward of ρ_0 through the transport plan, T.
- Quite challenging because of the constraint.

Kantorovich's formulation:

$$\inf_{\gamma \in \Pi(\rho_0, \rho_1)} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y)\, \gamma(dxdy).$$

- $\Pi(\rho_0, \rho_1) = \{\gamma \in P(\mathbb{R}^d \times \mathbb{R}^d) : \gamma_{\#}\pi_1 = \rho_0,\ \gamma_{\#}\pi_2 = \rho_1\}$.
- More generalized and easier to handle.
- The solution defines Wasserstein distance.

Interpolation

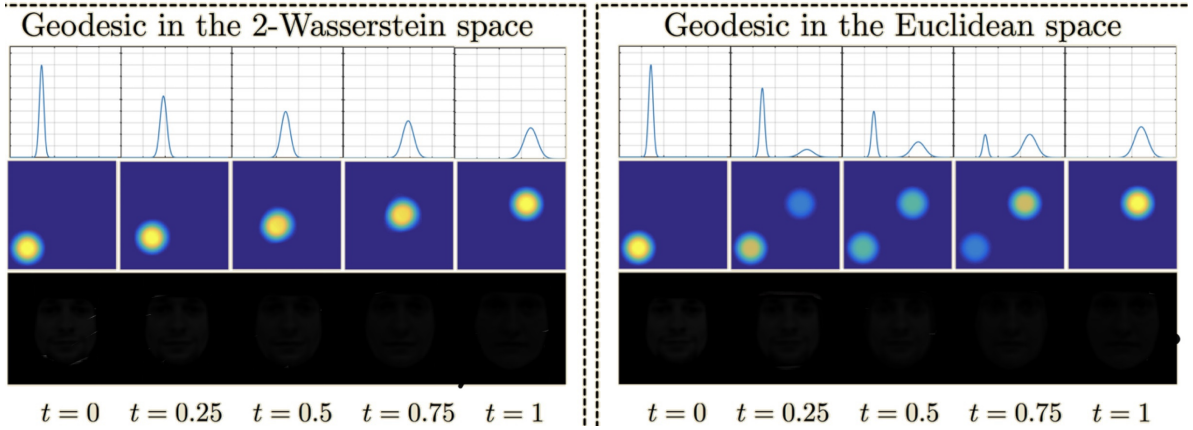
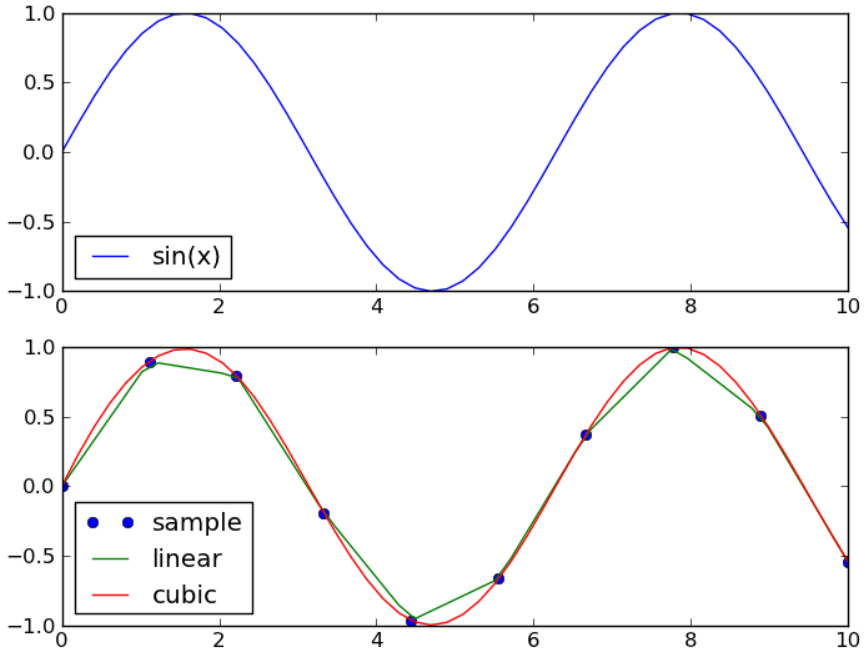


Figure: Interpolation between the optimal transport framework (left) and Euclidean space (right).

Wasserstein geodesic is essentially a "linear" distribution between distributions.

Linear interpolation vs Spline



Splines in $\mathbb{R}^d$

Definition 1

Let $\{t_i, x_i\}_{i=0}^N \subset [0,1] \times \mathbb{R}^d$ be give time-space data:

- A function $S \in C^2([0,1]; \mathbb{R}^d)$ is a **cubic spline** if S is a cubic polynomial in each interval $[t_i, t_{i+1}]$, $i = 0, \dots n$.
- A cubic spline is an **interpolating cubic spline** if $S_{t_i} = x_i$ for all $i = 0, 1, \dots, n$.
- An interpolating spline is called **natural** if $\partial_{tt} S_{t_0} = \partial_{tt} S_{t_1} = 0$.

WLOG, assume $0 = t_0 < t_1 < \cdots < t_N = 1$.

Aim: To use this concept to interpolate distributions smoothly.

Variational Interpretation

Theorem 2 (Holladay '57)

Let $\{t_i, x_i\}_{i=0}^N \subset [0,1] \times \mathbb{R}^d$ be given time-space data. The variational problem

$$\inf_X \int_0^1 |\partial_{tt} S_t|^2 \, dt,$$
$$X \in H^2([0,1]; \mathbb{R}^d),$$
$$X_{t_i} = x_i,$$

admits a unique solution, which is the natural interpolating spline.

$H^2([0,1]; \mathbb{R}^d)$ is the space of twice continuously differentiable functions with square-integrable second order derivative.

Natural cubic spline minimizes mean-squared acceleration!

Splines in $\mathcal{P}_2(\mathbb{R}^d)$

Spline Interpolation of Distributions

The problem of transporting mass configuration ρ_0 into the mass configuration ρ_i at time t_i while minimizing the mean squared acceleration.

- A **transport plan** P is a probability distribution on space $\Omega = C^0$.
- For $A \subset \Omega$, $P(A)$ represents the total mass that flows along the paths in A.

X_t is the projection map: $\forall \omega \in \Omega,\ X_t(\omega) = \omega_t$.

Definition 3

Let $\{t_i, \rho_i\}_{i=0}^N \subset [0,1] \times P_2(\mathbb{R}^d)$ be given data. The marginal flow ρ_t of an optimal solution of the problem

$$\begin{aligned} &\inf_P \int_0^1 \int_\Omega |\partial_{tt} X_t|^2 \, dP dt, \\ &P \in \mathcal{P}(\Omega),\ P(H^2) = 1, \\ &(X_{t_i})_\# P = \rho_i,\ i = 0, 1, \ldots, N, \end{aligned}$$

is an **interpolating spline** for the given data.

We can guarantee existence but not uniqueness.

Consistency

Proposition

Let $\{t_i, x_i\} \subset [0,1] \times \mathbb{R}^d$ and set $\rho_i := \delta_{x_i}$ for $0 \leq i \leq N$. Then the unique optimal solution is

$$P^* = \delta_S,$$

where S is the natural interpolating spline for $\{t_i, x_i\}_{i=0}^N$.

All the particles are tied to each other and move together

Existence

$X_{\mathcal{T}} := (X_{t_0}, X_{t_1}, \dots, X_{t_N})$,
$\Pi(\rho_0, \rho_1, \dots, \rho_N) = \{\pi \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d \dots \times \mathbb{R}^d) : (Y_i)_{\#}\pi = \rho_i\}$.

Theorem 4

Let $\{\rho_i\}_{i=0}^N \subset \mathcal{P}_2(\mathbb{R}^d)$. Then there exists at least an optimal solution to the problem. Moreover, the following are equivalent

(a) $\hat{P}$ is an optimal solution.

(b) $\hat{P}(\mathcal{S}_3^0) = 1$ and $\hat{\pi} := (X_{\mathcal{T}})_{\#}\hat{P}$ is an optimal solution for

$$\inf_{\pi} \int \mathcal{C}(x_0, x_1, \dots, x_N)\, d\pi,$$
$$\pi \in \Pi(\rho_0, \rho_1, \dots, \rho_N).$$

$$\mathcal{C}(x_0, x_1, \dots, x_N) = \int_0^1 |\partial_{tt} S_t(x_0, x_1, \dots, x_N)|^2\, dt.$$

- An optimal solution is supported on natural splines of $\mathbb{R}^d$.
- Its joint distribution at times $(t_0, t_1, \ldots, t_N)$ solves a multimarginal optimal transport problem whose cost function is $\mathcal{C}$.
- $\mathcal{C}(x_0, x_1 \ldots, x_N)$ is the optimal value as in the original variational problem in $\mathbb{R}^d$ (Mean-squared acceleration of natural spline).
- The spline thus obtained is analogous to the fact that the geodesics of $\mathcal{P}_2(\mathbb{R}^d)$ are constructed pushing forward the optimal coupling of the Monge-Kantorovich problem through geodesics of $\mathbb{R}^d$.
- This approach is computationally burdensome.

Formulation in phase space

Enlarge the space to $H^1 \times H^1$.

$$\begin{aligned}
&\inf_Q \int_0^1 \int_{\Omega\times\Omega} |\partial_t V_t|^2 \, dQdt, \\
&Q \in \mathcal{P}(\Omega \times \Omega), \;\; Q(H^1 \times H^1) = 1, \\
&Q(\partial_t X_t = V_t \; \forall t \in [0,1]) = 1, \\
&(X_{t_i})_\# Q = \rho_i, \;\; i = 0, 1, \ldots, N.
\end{aligned}$$

This is equivalent to the previous problem.

Analogous $\mathcal{C}$ has a closed form solution.

Fluid dynamical formulation

Monge-Kantorovich

Recall: Fluid dynamical formulation of the MP problem is due to Benamou and Brenier (2000). The optimal value for

$$\inf_{\mu,\nu} \int_0^1 \int_{\mathbb{R}^d} |\nu_t|^2(x)\mu_t(x)\, dxdt,$$
$$\partial_t \mu_t(x) + \nabla \cdot (\nu_t \mu_t)(x) = 0,$$
$$\mu_0 = \rho_0,\ \mu_1 = \rho_1.$$

is the squared Wasserstein distance $W_2^2(\rho_0, \rho_1)$ and the optimal curve is the displacement interpolation.

Splines

Problem:

$$\inf_{\mu,a} \int_0^1 \int_{\mathbb{R}^d} |a_t(x,\nu)|^2 \mu_t(x,\nu)\, dx d\nu,$$
$$\partial_t \mu_t(x,\nu) + \langle \nabla_x \mu_t(x,\nu), \nu \rangle + \nabla_\nu \cdot (a_t \mu_t)(x,\nu) = 0,$$
$$\int_{\mathbb{R}^d} \mu_{t_i}(x,\nu)\, d\nu = \rho_{t_i}, \quad i = 0, 1, \ldots, N.$$

This problem is equivalent to the variational form.

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Thank You!

Questions?