Collision-based Dynamics for Optimal Transport Problem with Application in Generative Models

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Optimal Transport Problem

Consider K probability measures $\mu^{(i)} \in \mathcal{P}_2(\mathcal{X}^{(i)})$ with $i \in \{1, ..., K\}$. The Multi-Marginal Optimal Transport problem (MMOT) seeks the optimal joint density π^* as the solution to the minimization problem

$$\pi^* := \underset{\pi \in \Pi(\mu^{(1)},...,\mu^{(K)})}{\arg\min} \int_{\mathcal{X}} c(x^{(1)}, ..., x^{(K)}) \pi(dx) \ , \qquad (1)$$

where $\mathcal{X}$ is the product set $\mathcal{X} := \mathcal{X}^{(1)} \times ... \times \mathcal{X}^{(K)}$, $\mathcal{P}(\mathcal{X}^{(i)})$ be the space of non-negative Borel measures over $\mathcal{X}^{(i)} \subset \mathbb{R}^n$, and

$$\mathcal{P}_2(\mathcal{X}^{(i)}) := \left\{ \mu \in \mathcal{P}(\mathcal{X}^{(i)}) \middle| \int_{\mathcal{X}^{(i)}} \|x\|_2^2 \mu(dx) < \infty \right\} \qquad (2)$$

with $\|.\|_2$ the L^2-Euclidean norm.

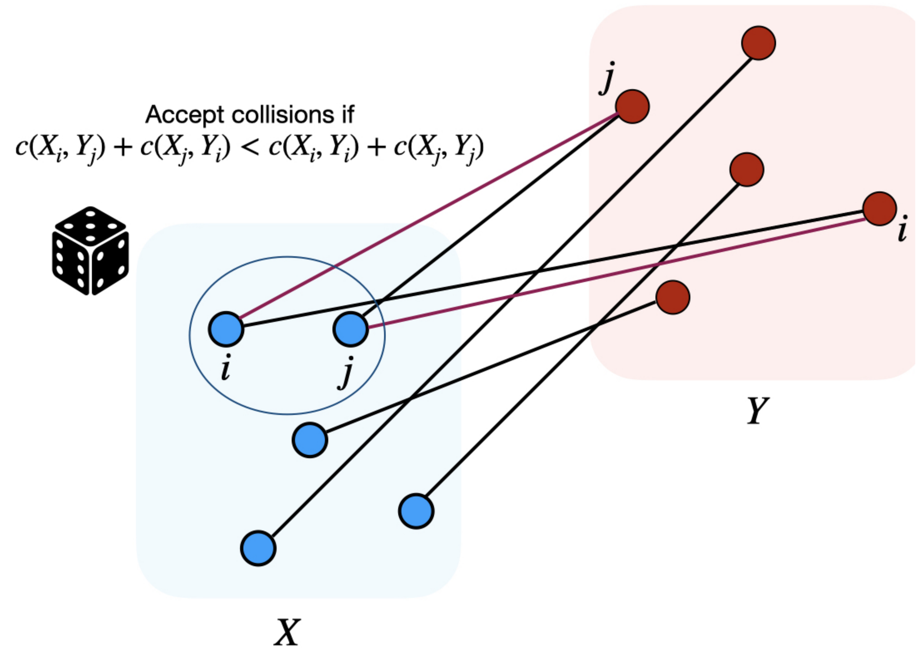
The MMOT optimization is constrained on the set of all couplings Π

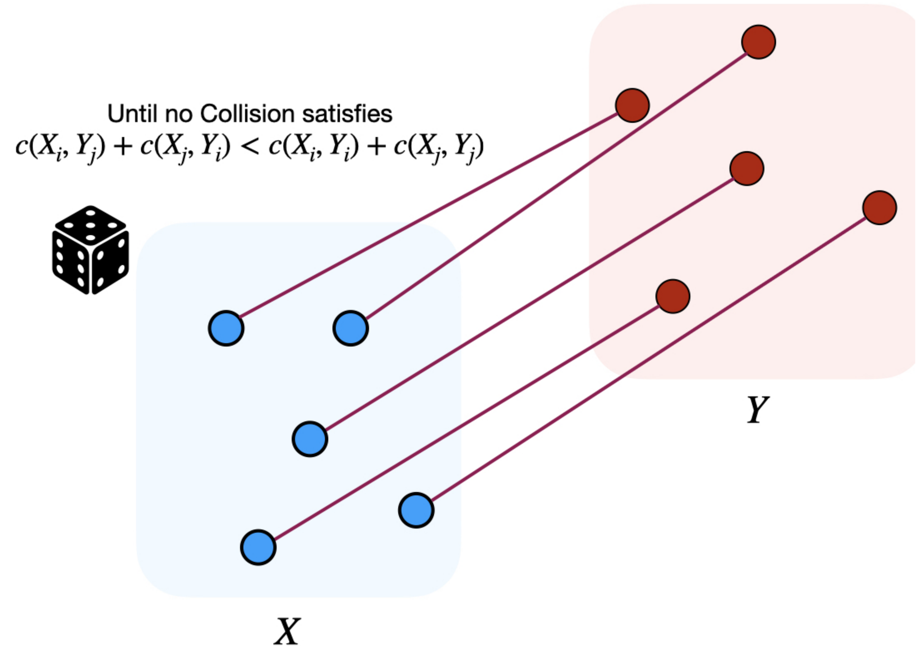
$$\Pi(\mu^{(1)}, ..., \mu^{(K)}) := \left\{ \pi \in \mathcal{P}_2(\mathcal{X}) \middle| \mathrm{proj}_i(\pi) = \mu^{(i)} \ \forall i \in \{1, ..., K\} \right\} \qquad (3)$$

and $\mathrm{proj}_i : \mathcal{X} \to \mathcal{X}^{(i)}$ is the canonical projection. For simplicity, here we consider

$$c(x^{(1)}, ..., x^{(K)}) = \sum_{i=1}^{K} \sum_{j=i+1}^{K} \frac{1}{2} \|x^{(i)} - x^{(j)}\|_2^2 \qquad (4)$$

as the cost function.





Iterated Swapping Algorithm (ISA)

ISA considers all the possible binary combinations, i.e. for each marginal $i \in \{1, ..., K\}$ and every pair of samples $j, k \in \{1, ..., N_p\}$ with $k \geq j$, swaps the particles

$$(X_{j,t+1}^{(i)}, X_{k,t+1}^{(i)})^T = \mathcal{K}_{j,k} (X_{j,t}^{(i)}, X_{k,t}^{(i)})^T. \qquad (5)$$

The swaps are guided by the discrete cost

$$m(\tilde{\pi}_t) = \mathbb{E}_{\tilde{\pi}_t}[c] \qquad (6)$$

where $\tilde{\pi}_t$ is the empirical measure of X_t. The swapping kernel is given by

$$\mathcal{K}_{j,k} = \begin{cases} I_{2n \times 2n} & \text{if } m(\tilde{\pi}_t^{X_j^{(i)} \leftrightarrow X_k^{(i)}}) \geq m(\tilde{\pi}_t) \\ J_{2n \times 2n} & \text{if } m(\tilde{\pi}_t^{X_j^{(i)} \leftrightarrow X_k^{(i)}}) < m(\tilde{\pi}_t) \end{cases} \qquad (7)$$

with $I_{n \times n}$ as the identity matrix and J an exchange matrix of the form

$$J_{2n \times 2n} = \begin{bmatrix} 0_{n \times n} & I_{n \times n} \\ I_{n \times n} & 0_{n \times n} \end{bmatrix} \qquad (8)$$

and $0_{n \times n}$ is a $n \times n$ matrix with zero entries.
Monotone Convergence, since swaps are only accepted if transport optimal cost is decreased.
Complexity of $\mathcal{O}(N_p^2)$ since all the pair-wise combinations are considered.

Exponential Convergence

Let us consider the Cauchy problem

$$\frac{\partial \rho}{\partial t} = P[\rho, \rho] - \hat{\alpha} \rho \qquad (11)$$

where $P[\rho, \rho]$ is a bilinear operator, and $\hat{\alpha} \neq 0$ is a constant. The solution to the Cauchy problem can be written as

$$\rho = e^{-\hat{\alpha} t} \sum_{k=0}^{\infty} (1 - e^{-\hat{\alpha} t})^k \rho_k \qquad (12)$$

where ρ_k is given by the recurrence formula

$$\rho_k = \frac{1}{k+1} \sum_{h=0}^{k} \frac{1}{\hat{\alpha}} P[\rho_h, \rho_{k-h}]. \qquad (13)$$

By defining $P[\rho, \rho] := Q[\rho, \rho] + \hat{\alpha} \rho$, formally we have $\lim_{k \to \infty} \rho_k = \lim_{t \to \infty} \rho = \rho^*$, where ρ^* is the equilibrium solution to the Boltzmann equation, i.e. the target sub-optimal joint density in this context. For a given ϵ and $t > t_0$, there exists finite n_0 and K where the Wild expansion is bounded $F^{P_r(n)}(x) < K$, such that

$$|\rho - \rho^*| < K n_0 e^{-\hat{\alpha} t_0} + \frac{2}{3} \epsilon e^{-\hat{\alpha} t} \sum_{n=1}^{\infty} (1 - e^{-\hat{\alpha} t})^{n-1} \ . \qquad (14)$$

Collision-based Dynamics

We propose a gradient-free collision process that evolves an initial joint measure similar to binary collisions in gas dynamics, where collisions refer to swapping of two particles.

Let ρ be the time dependent density of the joint measure. An equivalent collision operator of the Boltzmann-type can be described as

$$Q[\rho, \rho] = \sum_{i=1}^{K} Q^{(i)}[\rho, \rho] \qquad (9)$$

$$Q^{(i)}[\rho, \rho] = \int \left(\rho^{(i)}(x_1) \rho^{(i)}(y_1) - \rho^{(i)}(x) \rho^{(i)}(y) \right) \Omega^{(i)}(x, x_1, y, y_1) dy dx_1 dy_1 \qquad (10)$$

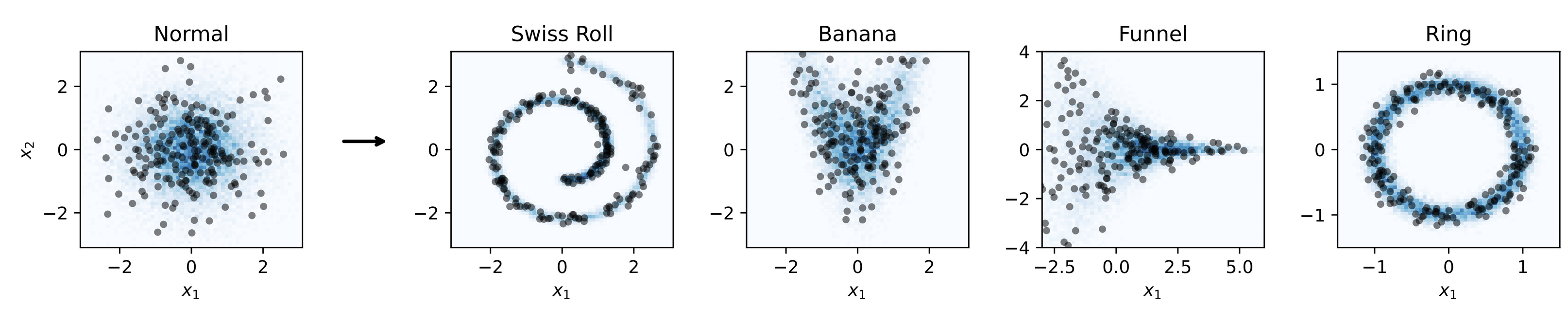
with the collision kernel

$$\Omega^{(i)}(x, x_1, y, y_1) = H\left(c(... \, x^{(i)} ...) + c(... \, y^{(i)} ...) - c(... \, x_1^{(i)} ...) - c(... \, y_1^{(i)} ...) \right)$$

where $H(.)$ is the Heaviside function.
Complexity of $\mathcal{O}(N_p)$ using direct Simulation Monte Carlo method.

Results

Sampling a five-marginal map.



Training Generative Model.

DDPM Collisional OT Loss

M. Sadr, H. Gorji. "Collision-based Dynamics for Multi-Marginal Optimal Transport." arXiv:2412.16385 (2025).

Code available on GitHub.