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 $\mathcal X:=\mathcal X^{(1)} imes ... imes \mathcal X^{(K)}$, $\mathcal P(\mathcal X^{(i)})$ be the space of nonnegative Borel measures over $\mathcal{X}^{(i)} \subset \mathbb{R}^n$, and

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

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

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

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

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

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

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

The swaps are guided by the discrete cost

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

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

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

$$(7)$$

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

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

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.

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

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

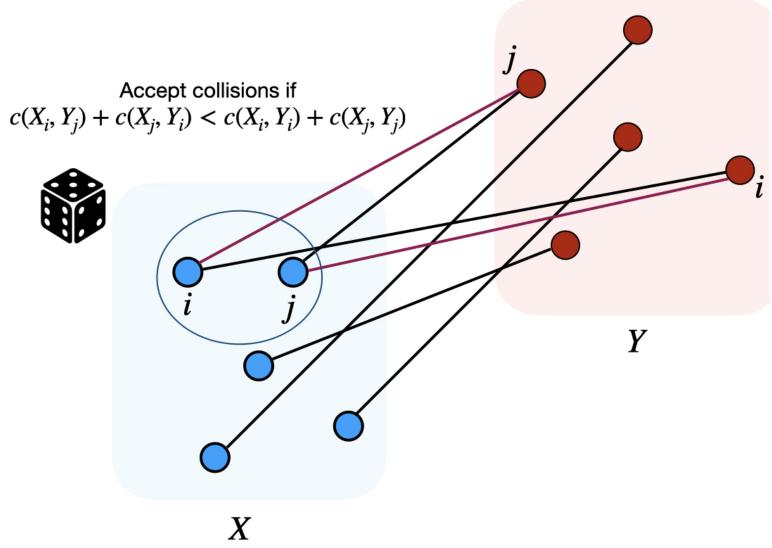
$$Q^{(i)}[\rho,\rho] = \int_{-\infty}^{i=1} \left(\rho^{(i)}(x_1)\rho^{(i)}(y_1) - \rho^{(i)}(x)\rho^{(i)}(y) \right) \Omega^{(i)}(x,x_1,y,y_1) dy dx_1 dy_1$$
 (10)

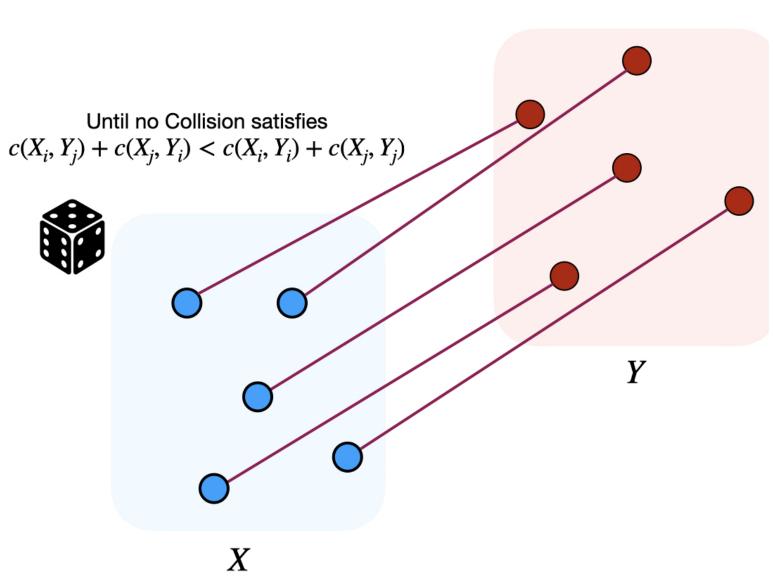
with the collision kernel

$$\Omega^{(i)}(x, x_1, y, y_1) = H\bigg(c(\dots x^{(i)}\dots) + c(\dots y^{(i)}\dots) - c(\dots x_1^{(i)}\dots) - c(\dots y_1^{(i)}\dots)\bigg)$$

where H(.) is the Heaviside function.

Complexity of $\mathcal{O}(N_p)$ using direct Simulation Monte Carlo method.





Exponential Convergence

Let us consider the Cauchy problem

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

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

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

where ρ_k is given by the recurrence formula

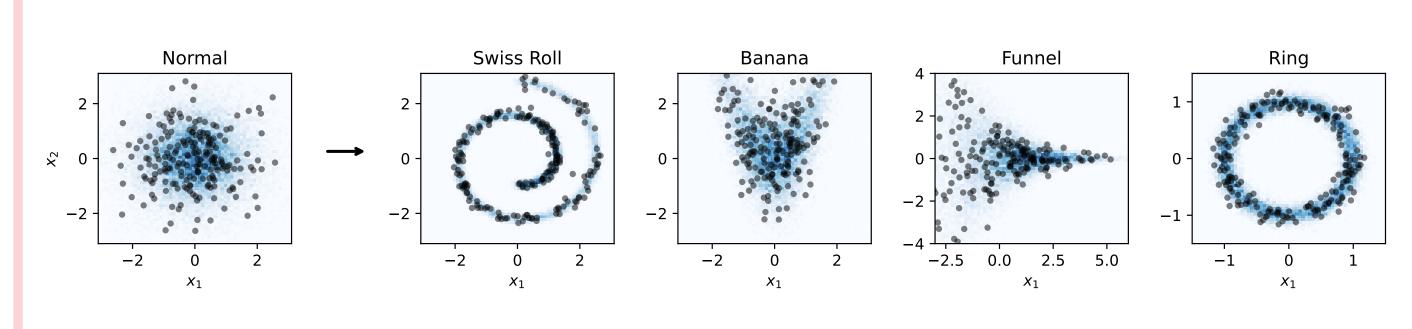
$$\rho_k = \frac{1}{k+1} \sum_{h=0}^{k} \frac{1}{\hat{\alpha}} P[\rho_h, \rho_{k-h}]. \tag{13}$$

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 suboptimal 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

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

Results

Sampling a five-marginal map.



Training Generative Model.

