Optimal Flow Matching: Straight trajectories in Flow Matching in just one step

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Goal of research

Main goal

Find a vector field u that describes ODE which effectively transports a given probability distribution p_0 to a target p_1.

Problems

Current methods obtain ODEs that have curved trajectories, resulting in time-consuming ODE integration for sampling.

Our solution

Look for the desired field in the class of specific field with straight trajectories by design.

Previous solutions

Flow Matching [Lipman et al., 2022]

Flow Matching Framework includes Diffusion models, score-based models, Optimal Transport and more.

Rectified Flow [Liu, 2022, Liu et al., 2022]

Iteratively solves FM and gradually rectifies trajectories. In each FM iteration, it **accumulates the error**.

Optimal Transport [Villani et al., 2009]

In OT, we move one probability distribution to another with the minimal effort. Such optimal transportations are usually described by ODEs with straight trajectories.

OT-Conditional Flow Matching [Pooladian et al., 2023]

Apply FM on top of optimal displacement between discrete batches from considered distributions. Such a heuristic does not actually guarantee straight paths because of **minibatch OT biases**.

Contributions

We propose a novel Optimal Flow Matching (OFM) approach that after a **single** FM iteration obtains straight trajectories which can be simulated without ODE solving. It recovers OT solution for the quadratic transport cost function.

Рис.: Comparison with other methods in unpaired ADULT to CHILD image translation

ODE preliminaries

Consider:

- Fixed time interval $[0, 1]$.
- Vector field $u(t, \cdot) \equiv u_t(\cdot) : [0, 1] \times \mathbb{R}^D \to \mathbb{R}^D$.
- Set of random trajectories s.t. for each trajectory $\{z_t\}_{t\in[0,1]}$ the starting point z_0 is sampled from p_0 and z_t satisfies the differential equation

$$dz_t = u_t(z_t)dt, \quad z_0 \sim p_0.$$

- $\phi^u(t, \cdot) \equiv \phi_t^u(\cdot) : [0, 1] \times \mathbb{R}^D \to \mathbb{R}^D$ is the function that maps the initial z_0 to its position at time t

Optimal Transport: Theory [Villani et al., 2009]

Consider

- Two absolutely continuous distributions p_0, p_1 in $\mathbb{R}^D$.
- Set of transport plans $\Pi(p_0, p_1)$, i.e., the set of joint distributions on $\mathbb{R}^D \times \mathbb{R}^D$ which marginals are equal to p_0 and p_1.
- The quadratic cost function $c(x_0, x_1) = \frac{\|x_1 - x_0\|^2}{2}$.

Dynamic Optimal Transport

$$\mathbb{W}_2^2(p_0, p_1) = \inf_u \quad \int_0^1 \int_{\mathbb{R}^D} \frac{\|u_t(x)\|_2^2}{2} \underbrace{\phi_t^u \# p_0(x)}_{:=p_t(x)} dxdt, \tag{1}$$

$$s.t. \qquad \phi_1^u \# p_0 = p_1.$$

For every initial point z_0, the solution defines a linear trajectory $\{z_t\}_{t\in[0,1]}$:

$$z_t = t\nabla\Psi^*(z_0) + (1-t)z_0, \quad \forall t \in [0,1], \tag{2}$$

where Ψ^* is a convex function.

Flow Matching: Theory [Lipman et al., 2022]

Consider two points x_0, x_1 sampled from a transport plan $\pi \in \Pi(p_0, p_1)$, e.g., the independent plan $p_0 \times p_1$. The vector field u is encouraged to follow the direction $x_1 - x_0$ of the linear interpolation $x_t = (1-t)x_0 + tx_1$ at any moment $t \in [0, 1]$.

Training objective:

$$
\begin{aligned}
\min_u \mathcal{L}_{FM}^{\pi}(u) \quad &:= \quad \int_0^1 \left\{ \int_{\mathbb{R}^D \times \mathbb{R}^D} \|u_t(x_t) - (x_1 - x_0)\|^2 \pi(x_0, x_1) dx_0 dx_1 \right\} dt \\
x_t \quad &= \quad (1-t)x_0 + tx_1.
\end{aligned}
$$

Optimal Vector Fields [Kornilov et al., 2024]

Optimal vector field u^Ψ generates linear trajectories $\{\{z_t\}_{t\in[0,1]}\}$ s.t. there exist a convex function $\Psi : \mathbb{R}^D \to \mathbb{R}$, which for any path $\{z_t\}_{t\in[0,1]}$ pushes the initial point z_0 to the final one as $z_1 = \nabla\Psi(z_0)$, i.e.,

$$z_t \quad = \quad (1-t)z_0 + t\nabla\Psi(z_0), \qquad t \in [0,1].$$

The formula $u_t^\Psi(x_t)$ for a time $t \in [0,1]$ and point x_t is constructed as follows: we can find a trajectory $\{z_t\}_{t\in[0,1]}$ s.t.

$$\begin{aligned} x_t \quad &= \quad (1-t)z_0 + t\nabla\Psi(z_0) \\ z_0^\Psi \quad &= \quad \arg\min_{z_0\in\mathbb{R}^D} \left[\frac{(1-t)}{2}\|z_0\|^2 + t\Psi(z_0) - \langle x_t, z_0\rangle\right] \\ u_t^\Psi(x_t) \quad &:= \quad \nabla\Psi(z_0^\Psi) - z_0^\Psi. \end{aligned}$$

Optimal Flow Matching: Theory [Kornilov et al., 2024]

We wish to construct a vector field u close to the OT field u^*:

$$\text{DIST}(u, u^*) := \int_0^1 \int_{\mathbb{R}^D} \|u_t(x_t) - u_t^*(x_t)\|^2 p_t^*(x_t) dx_t dt.$$

For arbitrary vector field u and OT field u^*:

$$\text{DIST}(u, u^*) = \mathcal{L}_{FM}^{\pi^*}(u) - \underbrace{\mathcal{L}_{FM}^{\pi^*}(u^*)}_{=0}.$$

We can not minimize intractable $\text{DIST}(u, u^*)$ since the optimal plan π^* is unknown. Surprisingly, for the *optimal* vector fields, the distance can be calculated explicitly via **any** known plan π:

$$\text{DIST}(u^\Psi, u^{\Psi^*}) = \mathcal{L}_{FM}^{\pi}(u^\Psi) - \mathcal{L}_{FM}^{\pi}(u^{\Psi^*}).$$

Optimal Flow Matching: Practice [Kornilov et al., 2024]

We minimize Flow Matching loss only over optimal vector fields. In that case, OFM loss has simplified form

$$\mathcal{L}^{\pi}_{OFM}(\Psi) = \mathcal{L}^{\pi}_{FM}(u^{\Psi}) = \int_0^1 \left\{ \int_{\mathbb{R}^D \times \mathbb{R}^D} \left\| \frac{z_0^{\Psi}(x_t) - x_0}{t} \right\|^2 \pi(x_0, x_1) dx_0 dx_1 \right\} dt$$

and gradient with constant $z_0 = z_0^{\Psi}(x_t)$

$$\frac{d\mathcal{L}^{\pi}_{OFM}}{d\theta} := \frac{d}{d\theta} \mathbb{E} \left\langle \text{NO-GRAD} \left\{ 2 \left(t\nabla^2 \Psi_{\theta}(z_0) + (1-t)I \right)^{-1} \frac{(x_0 - z_0)}{t} \right\}, \nabla \Psi_{\theta}(z_0) \right\rangle$$

Theorem (OFM and OT connection [Kornilov et al., 2024])

*Let us consider two distributions p_0, p_1 and **any** transport plan $\pi \in \Pi(p_0, p_1)$ between them. Then, minimization of $\mathcal{L}^{\pi}_{OFM}(\Psi)$ retrieves OT solution:*

$$\Psi^* \in \arg \min_{convex\ \Psi} \mathcal{L}^{\pi}_{OFM}(\Psi).$$

Experiments

We compare OFM with independent and minibatch OT plans, FM based approaches and OT solver MMv1 on OT benchmark. We measure similarity between obtained transport map and ground truth solution via $\mathcal{L}^2$−UVP metric. Convex functions are parametrized by Input Convex Neural Networks.

Solver	Solver type|DIM	$D=2$	$D=4$	$D=8$	$D=16$	$D=32$	$D=64$	$D=128$	$D=256$
MMv1	**OT solver**	0.2	1.0	1.8	1.4	6.9	8.1	2.2	2.6
OFM Ind 1024 **(Ours)**		0.51	—	—	2.71	—	10.98	16.78	—
OFM MB 64 **(Ours)**		—	—	—	—	—	—	—	—
OFM MB 1024 **(Ours)**		0.70	—	—	2.58	—	10.66	8.56	—
OT-CFM 64	**Flow Matching**	0.68	0.99	2.98	5.0	8.2	12.0	13.8	31.4
OT-CFM 1024		0.16	0.73	2.27	4.33	7.9	11.4	12.1	27.5
c-**RF**		1.56	13.11	17.87	35.39	48.46	66.52	68.08	76.48
RF		8.58	49.46	51.25	63.33	63.52	85.13	84.49	83.13
Linear	**Baseline**	14.1	14.9	27.3	41.6	55.3	63.9	63.6	67.4

Among FM-based methods, OFM with any plan demonstrates the best results in all dimensions. For all 3 plans, OFM convergences to close final solutions and metrics.

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