Optimal Flow Matching: Learning Straight Trajectories in Just One Step

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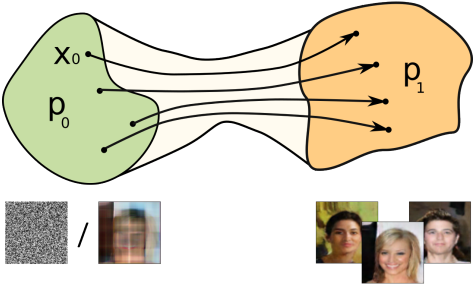
Goal of research

Main goal

Effectively map distribution p_0 to distribution p_1 via an ODE on $[0, 1]$

Challenges

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



Previous solutions

Flow Matching [Lipman et al., 2022]

Flow Matching Framework learns to the NN parametrized vector field of linear interpolation between p_0 and p_1. It includes Diffusion models and score-based models.

Optimal Transport [Villani et al., 2009]

OT moves one probability distribution to another with the minimal efforts. Such optimal transportation has ODE with straight trajectories.

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

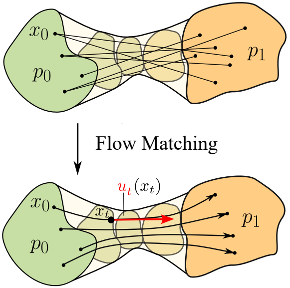
Apply FM on top of optimal displacement between discrete batches from considered distributions. Such a heuristic does not actually guarantee straight paths because of **minibatch OT biases**.

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

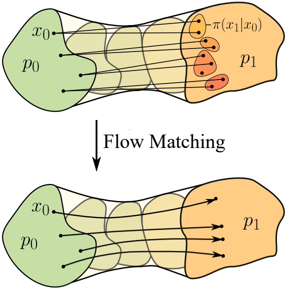
Iteratively solves FM and gradually rectifies trajectories. In practice, it **accumulates the error** with each iteration.

Previous solutions: FM and OT-CFM

Flow Matching

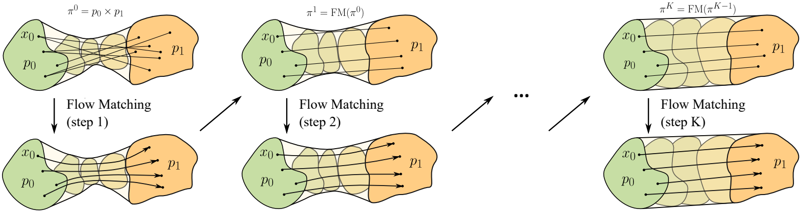


Optimal Transport between batches

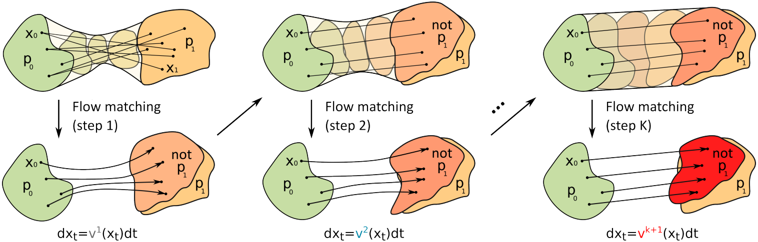


Previous solutions: RF

In theory:

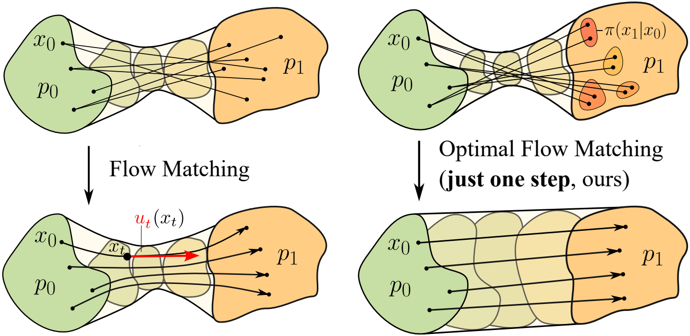


In practice:



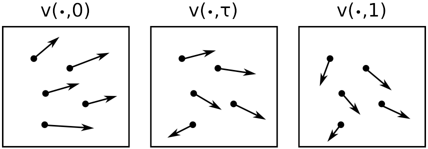
Contributions

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



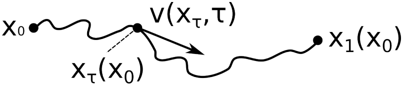
ODE preliminaries

Vector field $\upsilon : \mathbb{R}^D \times [0,1] \to \mathbb{R}^D$.



Movement of a point along the field. Let $x_t(x_0)$ be the solution to $x_t = \upsilon(x_t, t)t$ with initial condition $x_{t=0} = x_0$, i.e.:

$$x_t(x_0) = x_0 + \int_0^t \upsilon(x_\tau(x_0), \tau)\tau.$$



$\phi^u(t,\cdot) \equiv \phi^u_t(\cdot) : [0,1] \times \mathbb{R}^D \to \mathbb{R}^D$ is a function that maps an initial x_0 to its position at time t

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

Consider

- 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

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

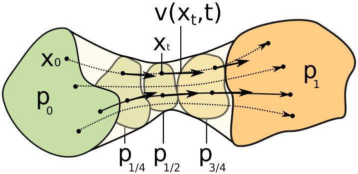
$$s.t. \quad \phi_1^u \# p_0 = p_1.$$

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

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

where Ψ^* is a convex function.

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

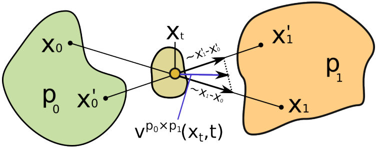


$$\begin{cases} x_t = v(x_t, t)t \\ x_0 \sim p_0 \end{cases}$$

Build linear interpolation probability path $p_t : x_t = x_0 \cdot (1-t) + x_1 \cdot t$, where x_0, x_1 are sampled from transport plan $\pi \in \Pi(p_0, p_1)$.

This probability path is generated by a solution to Flow Matching (FM) objective:

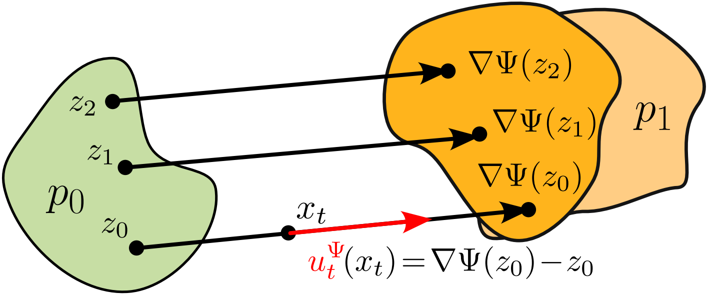
$$\boxed{\min_{v} \mathop{\mathbb{E}}_{x_0, x_1 \sim \pi} \left\{ \mathop{\mathbb{E}}_{t \sim [0,1]} \left\| \underset{x_0 \cdot (1-t) + x_1 \cdot t}{v(\underset{\|}{x_t}, t)} - (x_1 - x_0) \right\|^2 \right\}.}$$



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.,

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



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

Optimal Flow Matching [Kornilov et al., 2024]

Main idea: minimize Flow Matching loss only over optimal vector fields:

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

OFM loss has gradient:

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

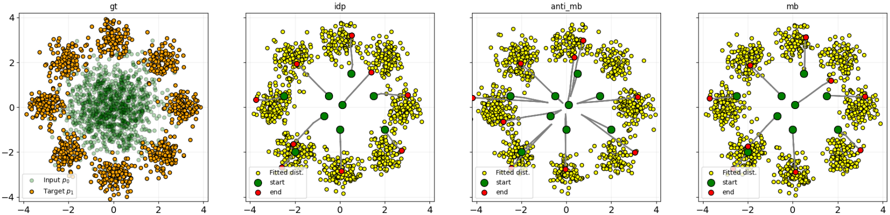
Theorem (OFM and OT connection [Kornilov et al., 2024])

*Consider two distributions p_0, p_1 and **any** transport plan $\pi \in \Pi(p_0, p_1)$ between them. Minimization of $\mathcal{L}^{\pi}_{OFM}(\Psi)$ retrieves the same OT solution with exactly straight paths:*

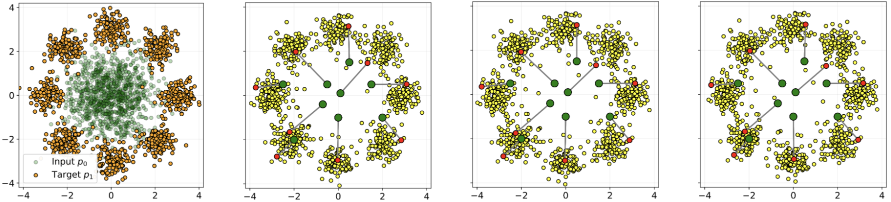
$$\Psi^* \in \arg \min_{convex\ \Psi} \mathcal{L}^{\pi}_{OFM}(\Psi).$$

Experiments: theory back up

Flow Matching:



Optimal Flow Matching:



(a) Input and target (b) Independent π (c) **Anti**minibatch π (d) Minibatch π

Experiments: OT benchmarks

Method	OFM, Ind **(Ours)**	OFM, MB **(Ours)**	RF
FID	11.8	**11.0**	21.0

On OT benchmark, **OFM demonstrates SOTA results.**

References

Kornilov, N., Gasnikov, A., and Korotin, A. (2024).
Optimal flow matching: Learning straight trajectories in just one step.
arXiv preprint arXiv:2403.13117.

Lipman, Y., Chen, R. T., Ben-Hamu, H., Nickel, M., and Le, M. (2022).
Flow matching for generative modeling.
arXiv preprint arXiv:2210.02747.

Liu, Q. (2022).
Rectified flow: A marginal preserving approach to optimal transport.
arXiv preprint arXiv:2209.14577.

Liu, X., Gong, C., and Liu, Q. (2022).
Flow straight and fast: Learning to generate and transfer data with rectified flow.
arXiv preprint arXiv:2209.03003.

Pooladian, A.-A., Ben-Hamu, H., Domingo-Enrich, C., Amos, B., Lipman, Y., and Chen, R. T. Q. (2023).
Multisample flow matching: Straightening flows with minibatch couplings.

Villani, C. et al. (2009).
Optimal transport: old and new, volume 338.
Springer.