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Optimal Flow Matching: Learning Straight Trajectories in Just One Step

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GitHub

I Background: Flow Matching[1]

Given two probability distributions source p_0 and target p_1, how to transform p_0 to p_1 via an ODE?

ODE with the vector field u takes the initial point x_0 and moves it according to

$$dx_t = u_t(x_t)dx_t, \quad x_0 \sim p_0, \quad t \in [0,1]$$

For a transport plan $\pi \in \Pi(p_0, p_1)$, we can obtain the target via

$$x_t = (1-t)x_0 + tx_1, \quad (x_0, x_1) \sim \pi$$

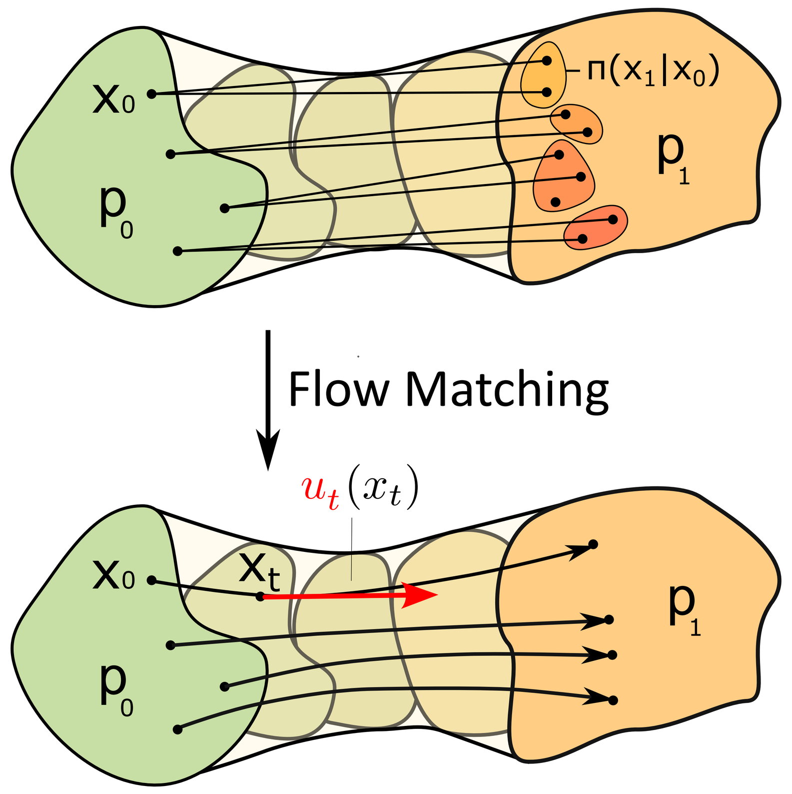
This equation is described by the *conditioned* vector field

$$v_t(x_t|x_1) = x_1 - \frac{x_t - tx_1}{1-t} = x_1 - x_0$$

Flow Matching (FM) finds the closest to v *unconditioned* vector field u:

$$\mathcal{L}^{\pi}_{FM}(u) := \int_0^1 \left\{ \int_{\mathbb{R}^d \times \mathbb{R}^d} ||u_t(x_t) - (x_1 - x_0)||^2 \pi(x_0, x_1) dx_0 dx_1 \right\} dt$$

$$FM(\pi) = \underset{u}{\operatorname{argmin}} \, \mathcal{L}^{\pi}_{FM}(u)$$



II Background: Rectified Flow[2]

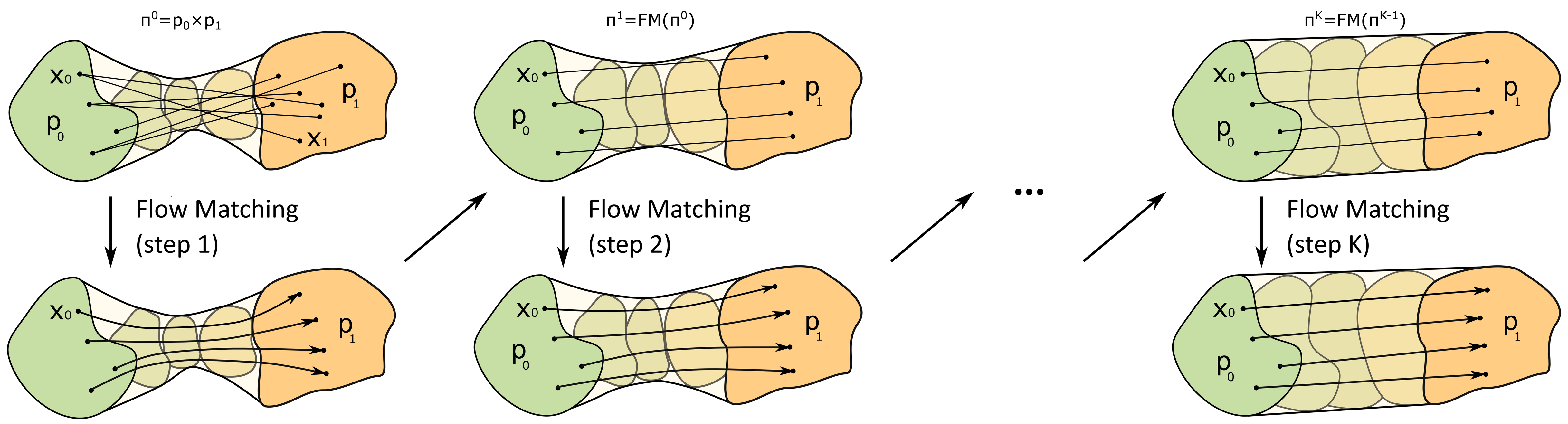
Main issue: FM generates curved trajectories.

Straightness is crucial for fast sampling of diffusion models.

Some initial plans π may cause more straight trajectories, e.g., mini batch plan from OT-CFM[3].

However, after FM minimization, the curvature of the obtained paths decreases.
Rectified Flow (RF): iteratively apply FM gradually straightening trajectories:

$$\pi^{K+1} = FM(\pi^K), \quad \pi^0 = \pi, \quad K = 0, 1, \ldots$$

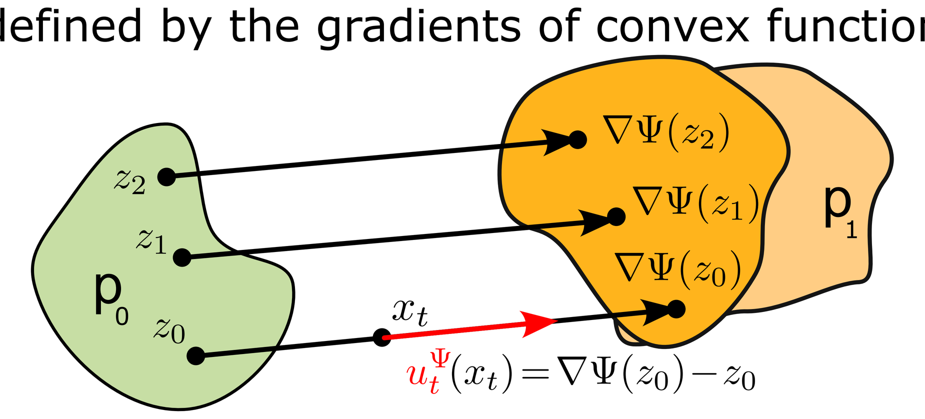


Main drawback: RF requires **several** expensive FM minimizations and **accumulates error** failing to capture the target.

III Optimal Flow Matching: Theory

Optimal vector fields

generate exactly straight paths. They are defined by the gradients of convex functions



$$x_t = (1-t)z_0 + t\nabla\Psi(z_0)$$

These fields are typical for the solutions of Optimal Transport (OT).

Main idea

minimize FM loss ***only over optimal fields***.

Our OFM Loss:

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

$$x_t = (1-t)x_0 + tx_1$$

For **any** plan π, minimization of OFM loss over Ψ recovers the vector field $\Psi^* = \arg\min_{\Psi} \mathcal{L}^{\pi}_{OFM}(\Psi)$ with **exactly straight** paths moving source to target.

Ψ^* is the solution of the OT with the quadratic cost between p_0 and p_1

IV Practical Algorithm

Implementation details

1) We parametrize the class of convex functions with Input Convex Neural Networks (ICNN)[4]

2) We use loss from line 6 which has the same gradients as our original OFM loss.

3) To solve strony convex minimization from line 5, we use LBFGS solver

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

Algorithm 1 Optimal Flow Matching

Input: Initial transport plan $\pi \in \Pi(p_0, p_1)$, number of iterations K, batch size B, optimizer Opt, sub-problem optimizer $SubOpt$, ICNN Ψ_θ

1: **for** $k = 0, \ldots, K-1$ **do**
2: Sample batch $\{(x^i_0, x^i_1)\}^B_{i=1}$ of size B from plan π;
3: Sample times batch $\{t^i\}^B_{i=1}$ of size B from $U[0,1]$;
4: Calculate linear interpolation $x^i_{t^i} = (1-t^i)x^i_0 + t^i x^i_1$ for all $i \in \overline{1, B}$;
5: Find the initial points z^i_0 via solving the convex problem with $SubOpt$:

$$z^i_0 = \text{NO-GRAD}\left\{ \arg\min_{z^i_0} \left[\frac{(1-t^i)}{2} \|z^i_0\|^2 + t^i \Psi_\theta(z^i_0) - \langle x^i_{t^i}, z^i_0 \rangle \right] \right\};$$

6: Calculate loss $\hat{\mathcal{L}}_{OFM}$

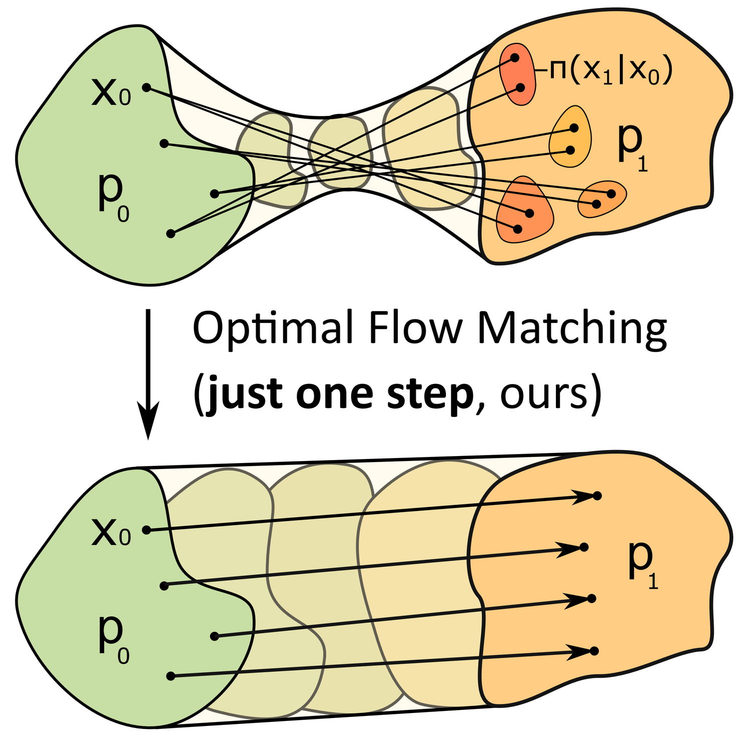
$$\hat{\mathcal{L}}_{OFM} = \frac{1}{B} \sum_{i=1}^{B} \left\langle \text{NO-GRAD}\left\{ 2\left(t^i \nabla^2 \Psi_\theta(z^i_0) + (1-t^i)I\right)^{-1} \frac{(x^i_0 - z^i_0)}{t^i} \right\}, \nabla\Psi_\theta(z^i_0) \right\rangle;$$

7: Update parameters θ via optimizer Opt step with $\frac{d\hat{\mathcal{L}}_{OFM}}{d\theta}$;
8: **end for**

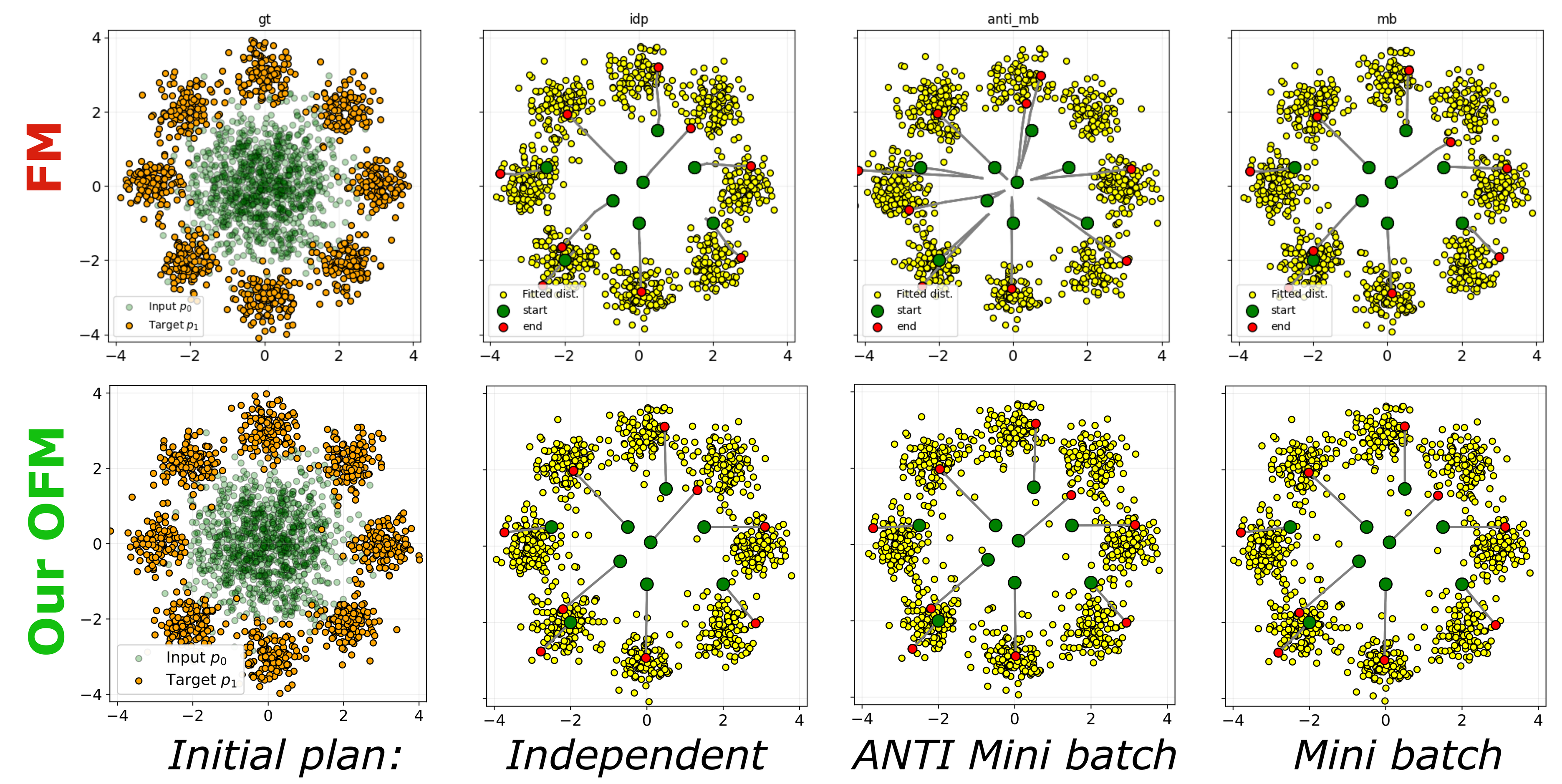
V Toy examples: FM and OFM

Mini batch: take batch and rearrange it to have **minimal** total pairwise distance.

ANTI Mini batch: take batch and rearrange to have **maximal** total pairwise distance.



Qualitative results of our OFM and original FM applied to 2D model distributions ("Gaussian" to "8 Gaussian").



Our OFM retrieves *the same* straight trajectories for all initial plans.

VI Unpaired Image-to-Image Translation

Qualitative results of our solver for solving the domain translation problem (in the latent space of the ALAE autoencoder).

Images resolution is 1024x1024.

1) OFM pairs have huge input-output similarity, since OFM implicitly solves Optimal Transport between domains.

2) Due to stochasticity during training, inital plan with straighter paths (MB) causes slightly better final translation.

References

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