

FLOW MATCHING FOR GENERATIVE MODELING

IDEA Seminar

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April 15, 2026

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CONTINUOUS NORMALIZING FLOWS

Let $\mathbf{x}^* \in \mathbb{R}^d$ be a random vector with density q .

Goal : Transform a simple distribution p_0 into a distribution p_1 that approximates q .

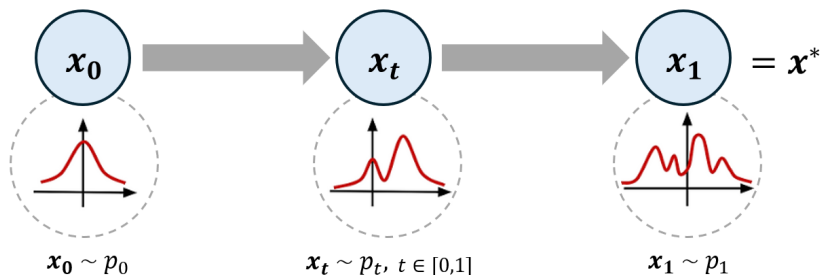


Figure. Overview of continuous normalizing flow

- ▶ Flow $\phi_t(\mathbf{x}) : [0, 1] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$, $\phi_0(\mathbf{x}_0) = \mathbf{x}_0$, $\phi_t(\mathbf{x}_0) = \mathbf{x}_t$
- ▶ Vector field $\mathbf{v}_t(\mathbf{x}) : [0, 1] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$, $\frac{d}{dt}\phi_t(\mathbf{x}) = \mathbf{v}_t(\phi_t(\mathbf{x}))$
- ▶ Model $\mathbf{v}_t(\mathbf{x})$ with a neural network $\mathbf{v}_t(\mathbf{x}; \theta)$, where $\theta \in \mathbb{R}^p$ are learnable parameters.

CONTINUOUS NORMALIZING FLOWS

Learn θ by minimizing the negative log-likelihood.

$$\begin{aligned}\mathcal{L}_{CNF}(\theta) &= \mathbb{E}[-\log p_1(\mathbf{x}_1)] \\ &= \mathbb{E}\left[-\log p_0(\mathbf{x}_0) + \int_0^1 \text{Tr}\left(\frac{\partial \mathbf{v}_t}{\partial \mathbf{x}}(\mathbf{x}_t; \theta)\right) dt\right]\end{aligned}$$

- ▶ Requires solving the following ordinary differential equation (ODE) to obtain \mathbf{x}_1 from \mathbf{x}_0 :

$$\frac{d\mathbf{x}_t}{dt} = \mathbf{v}_t(\mathbf{x}_t).$$

- ▶ Requires iterative computation while updating θ .
- ▶ Training is computationally expensive.

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METHOD

- ▶ Regression task by specifying a vector field $\mathbf{u}_t(\mathbf{x})$ and the corresponding probability path $p_t(\mathbf{x})$.

$$\mathcal{L}_{FM}(\theta) = \mathbb{E}_{t, p_t(\mathbf{x})} \|\mathbf{v}_t(\mathbf{x}; \theta) - \mathbf{u}_t(\mathbf{x})\|^2, \text{ where } t \sim U[0, 1].$$

- ▶ p_t and \mathbf{u}_t can be constructed using probability paths and vector fields defined for each sample of \mathbf{x}_1 .

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x} | \mathbf{x}_1) q(\mathbf{x}_1) d\mathbf{x}_1 \quad (1)$$

$$\mathbf{u}_t(\mathbf{x}) = \int \mathbf{u}_t(\mathbf{x} | \mathbf{x}_1) \frac{p_t(\mathbf{x} | \mathbf{x}_1) q(\mathbf{x}_1)}{p_t(\mathbf{x})} d\mathbf{x}_1 \quad (2)$$

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METHOD

- ▶ Then minimizing \mathcal{L}_{FM} is equal with minimizing

$$\mathcal{L}_{CFM}(\boldsymbol{\theta}) = \mathbb{E}_{t, q(\mathbf{x}_1), p_t(\mathbf{x}|\mathbf{x}_1)} \|\mathbf{v}_t(\mathbf{x}; \boldsymbol{\theta}) - \mathbf{u}_t(\mathbf{x} | \mathbf{x}_1)\|^2, \text{ where } t \sim U[0, 1].$$

Theorem 1

Assuming that $p_t(\mathbf{x}) > 0$ for all $\mathbf{x} \in \mathbb{R}^d$ and $t \in [0, 1]$, then, up to a constant independent of $\boldsymbol{\theta}$, \mathcal{L}_{CFM} and \mathcal{L}_{FM} are equal. Hence, $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{FM} = \nabla_{\boldsymbol{\theta}} \mathcal{L}_{CFM}$.

- ▶ Therefore, Now we need to design suitable $\mathbf{u}_t(\mathbf{x}|\mathbf{x}_1)$ and $p_t(\mathbf{x} | \mathbf{x}_1)$.

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DESIGNING CONDITIONAL PROBABILITY PATHS AND VECTOR FIELDS

- ▶ Consider Gaussian conditional probability paths.

$$p_t(\mathbf{x} \mid \mathbf{x}_1) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_t(\mathbf{x}_1), \sigma_t(\mathbf{x}_1)^2 I), \quad (3)$$

where $\boldsymbol{\mu} : [0, 1] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$, $\sigma : [0, 1] \times \mathbb{R}^d \rightarrow \mathbb{R}^+$, and I denote the identity matrix.

- ▶ Set $\boldsymbol{\mu}_0(\mathbf{x}_1) = 0$ and $\sigma_0(\mathbf{x}_1) = 1$, to make $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid 0, I)$.
- ▶ Consider the flow

$$\phi_t(\mathbf{x}) = \sigma_t(\mathbf{x}_1)\mathbf{x} + \boldsymbol{\mu}_t(\mathbf{x}_1). \quad (4)$$

- ▶ Then the corresponding vector field is

$$\frac{d}{dt}\phi_t(\mathbf{x}) = \mathbf{u}_t(\phi_t(\mathbf{x}) \mid \mathbf{x}_1).$$

Theorem 2

Let $p_t(\mathbf{x} \mid \mathbf{x}_1)$ be a Gaussian probability path as in equation (3), and ϕ_t its corresponding flow map as in equation (4). Then, the unique vector field that defines ϕ_t has the form:

$$\mathbf{u}_t(\mathbf{x} \mid \mathbf{x}_1) = \frac{\sigma'_t(\mathbf{x}_1)}{\sigma_t(\mathbf{x}_1)}(\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{x}_1)) + \boldsymbol{\mu}'_t(\mathbf{x}_1),$$

where $f' = \frac{d}{dt}f$. Consequently, $\mathbf{u}_t(\mathbf{x} \mid \mathbf{x}_1)$ generates the Gaussian path $p_t(\mathbf{x} \mid \mathbf{x}_1)$.

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DESIGNING CONDITIONAL PROBABILITY PATHS AND VECTOR FIELDS

Example 1: Diffusion conditional vector fields

Use diffusion paths as conditional probability paths in Flow Matching.

- ▶ **Flow Matching recovers diffusion dynamics.**
- ▶ Reversed (noise \rightarrow data) variance exploding diffusion path

$$p_t(\mathbf{x} \mid \mathbf{x}_1) = \mathcal{N}(\mathbf{x} \mid \mathbf{x}_1, s_{1-t}^2 l),$$

where s_t is an increasing function, $s_0 = 0$, and $s_1 \gg 1$.

$$\mathbf{u}_t(\mathbf{x} \mid \mathbf{x}_1) = -\frac{s'_{1-t}}{s_{1-t}}(\mathbf{x} - \mathbf{x}_1).$$

- ▶ Reversed (noise \rightarrow data) variance preserving diffusion path

$$p_t(\mathbf{x} \mid \mathbf{x}_1) = \mathcal{N}(\mathbf{x} \mid \alpha_{1-t}\mathbf{x}_1, (1 - \alpha_{1-t}^2)l),$$

where $\alpha_t = e^{-\frac{1}{2}T(t)}$, $T(t) = \int_0^t \beta$, and β is the noise scale function.

$$\mathbf{u}_t(\mathbf{x} \mid \mathbf{x}_1) = \frac{\alpha'_{1-t}}{1 - \alpha_{1-t}^2}(\alpha_{1-t}\mathbf{x} - \mathbf{x}_1).$$

FLOW MATCHING

DESIGNING CONDITIONAL PROBABILITY PATHS AND VECTOR FIELDS

Example 2: Optimal Transport (OT) conditional vector fields

Define the mean and the standard deviation to simply change linearly in time.

$$\mu_t(\mathbf{x}) = t\mathbf{x}_1, \quad \sigma_t(\mathbf{x}) = 1 - (1 - \sigma_{min})t,$$

where σ_{min} is a small constant representing the minimum noise level.

$$\mathbf{u}_t(\mathbf{x} | \mathbf{x}_1) = \frac{\mathbf{x}_1 - (1 - \sigma_{min})\mathbf{x}}{1 - (1 - \sigma_{min})t}.$$

- ▶ \mathbf{x}_t moves in straight line with constant speed, leading to more efficient computation.

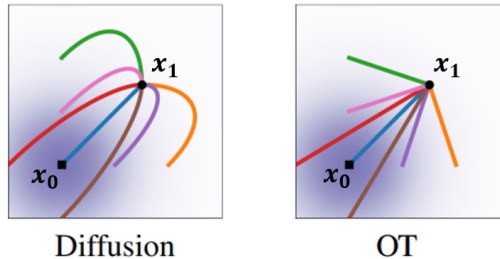


Figure. Diffusion and OT paths

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EXPERIMENTS

1. Density modeling and sample quality
2. Sampling efficiency
3. Conditional sampling from low-resolution images

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EXPERIMENTS

Density modeling and sample quality

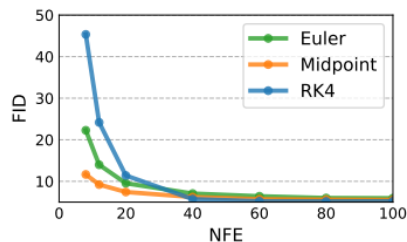
Model	CIFAR-10			ImageNet 32×32			ImageNet 64×64			Model	ImageNet 128×128	
	NLL↓	FID↓	NFE↓	NLL↓	FID↓	NFE↓	NLL↓	FID↓	NFE↓		NLL↓	FID↓
<i>Ablations</i>												
DDPM	3.12	7.48	274	3.54	6.99	262	3.32	17.36	264	MGAN (Hoang et al., 2018)	–	58.9
Score Matching	3.16	19.94	242	3.56	5.68	178	3.40	19.74	441	PacGAN2 (Lin et al., 2018)	–	57.5
ScoreFlow	3.09	20.78	428	3.55	14.14	195	3.36	24.95	601	Logo-GAN-AE (Sage et al., 2018)	–	50.9
<i>Ours</i>												
FM ^w / Diffusion	3.10	8.06	183	3.54	6.37	193	3.33	16.88	187	Self-cond. GAN (Lučić et al., 2019)	–	41.7
FM ^w / OT	2.99	6.35	142	3.53	5.02	122	3.31	14.45	138	Uncond. BigGAN (Lučić et al., 2019)	–	25.3
										PGMGAN (Armandpour et al., 2021)	–	21.7
										FM ^w / OT	2.90	20.9

Figure. Likelihood (BPD), quality of generated samples (FID), and evaluation time (NFE) for the same model trained with different methods.

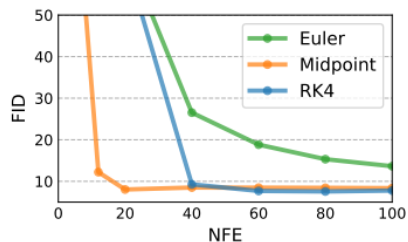
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EXPERIMENTS

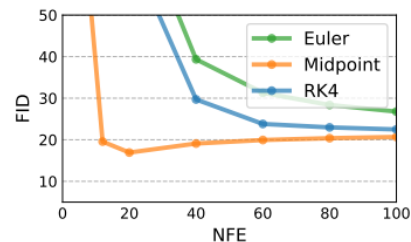
Sampling efficiency



Flow matching ^w/ OT



Flow matching ^w/ Diffusion



Score matching ^w/ Diffusion

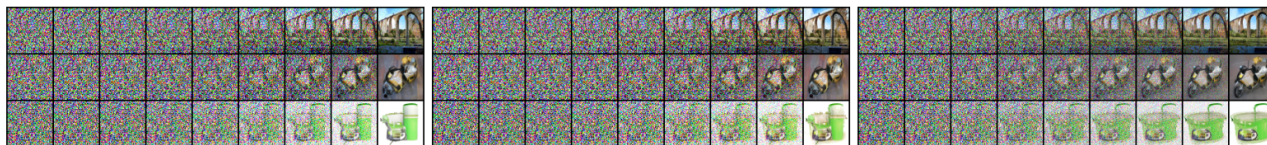
Figure. FID score and evaluation time for the models trained on ImageNet 32×32 .

- ▶ Flow Matching, especially when using OT paths, allows us to use fewer evaluations for sampling while retaining similar sample quality.

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EXPERIMENTS

Sampling efficiency



Score Matching w/ Diffusion

Flow Matching w/ Diffusion

Flow Matching w/ OT

Figure. Sample paths from the same initial noise with models trained on ImageNet 64×64 .

- ▶ The OT path reduces noise roughly linearly, while diffusion paths visibly remove noise only towards the end of the path.
- ▶ Note also the differences between the generated images.

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EXPERIMENTS

Conditional sampling from low-resolution images

Model	FID↓	IS↑	PSNR↑	SSIM↑
Reference	1.9	240.8	–	–
Regression	15.2	121.1	27.9	0.801
SR3 (Saharia et al., 2022)	5.2	180.1	26.4	0.762
FM ^w /OT	3.4	200.8	24.7	0.747

Figure. Image super-resolution on the ImageNet validation set.



Figure. Conditional generation $64 \times 64 \rightarrow 256 \times 256$. Flow Matching OT upsampled images from validation set.

Thank You

INDUCING NEGATIVE LOG-LIKELIHOOD

Let $J_t = \frac{\partial \mathbf{x}_t}{\partial \mathbf{x}_0}$ be the Jacobian. The log-density is $\log p_t(\mathbf{x}_t) = \log p_0(\mathbf{x}_0) - \log \det J_t$.

By the chain rule,

$$\frac{dJ_t}{dt} = \frac{\partial}{\partial \mathbf{x}_0} \left(\frac{d\mathbf{x}_t}{dt} \right) = \frac{\partial \mathbf{v}_t(\mathbf{x}_t)}{\partial \mathbf{x}_0} = \frac{\partial \mathbf{v}_t(\mathbf{x}_t)}{\partial \mathbf{x}_t} \frac{\partial \mathbf{x}_t}{\partial \mathbf{x}_0} = \left(\frac{\partial \mathbf{v}_t}{\partial \mathbf{x}_t} \right) J_t$$

Since the derivative of a log-determinant is given by $\frac{d}{dt} \log \det A_t = \text{Tr} \left(A_t^{-1} \frac{dA_t}{dt} \right)$.

Substituting J_t for A_t ,

$$\frac{d}{dt} \log \det J_t = \text{Tr} \left(J_t^{-1} \frac{dJ_t}{dt} \right) = \text{Tr} \left(J_t^{-1} \left(\frac{\partial \mathbf{v}_t}{\partial \mathbf{x}_t} \right) J_t \right) = \text{Tr} \left(\frac{\partial \mathbf{v}_t}{\partial \mathbf{x}_t} \right),$$

where the last step uses the cyclic property of the Trace ($\text{Tr}(ABC) = \text{Tr}(BCA)$).

Therefore,

$$\frac{d}{dt} \log p_t(\mathbf{x}_t) = -\text{Tr} \left(\frac{\partial \mathbf{v}_t}{\partial \mathbf{x}_t}(\mathbf{x}_t) \right)$$