

Deep Generative Models

Lecture 13

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Recap of Previous Lecture

Flow Matching (FM)

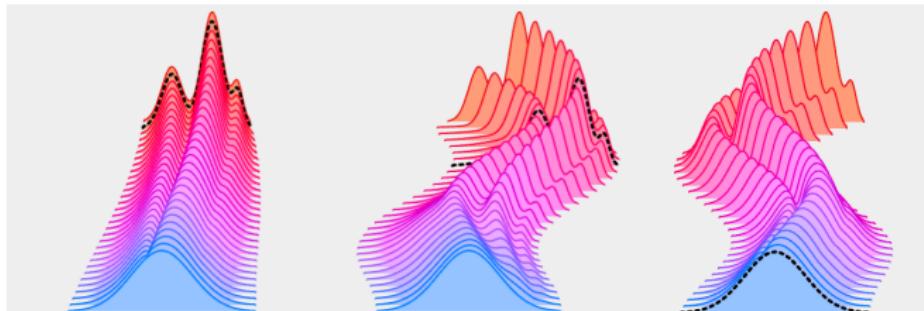
$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \|\mathbf{f}(\mathbf{x}, t) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

Conditional Flow Matching (CFM)

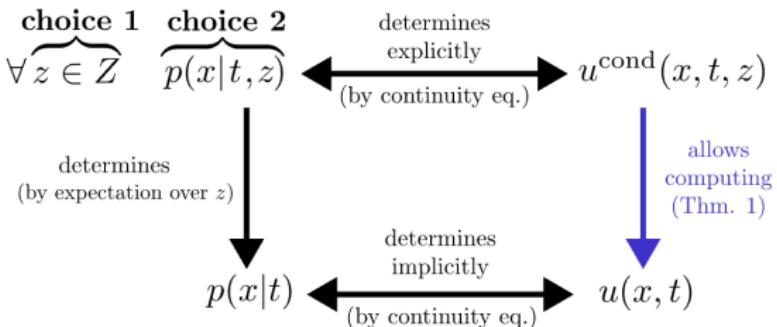
$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \|\mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

Theorem

If $\text{supp}(p_t(\mathbf{x})) = \mathbb{R}^m$, then the optimal value of the FM objective equals the optimum for CFM.



Recap of Previous Lecture



Constraints

$$p(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}) = \mathbb{E}_{p(\mathbf{z})} p_0(\mathbf{x}|\mathbf{z}); \quad p_{\text{data}}(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_1(\mathbf{x}|\mathbf{z}).$$

- ▶ How should we choose the conditioning latent variable \mathbf{z} ?
- ▶ How can we define $p_t(\mathbf{x}|\mathbf{z})$ so that it meets the constraints?

Gaussian Conditional Probability Path

$$p_t(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_t(\mathbf{z}), \boldsymbol{\sigma}_t^2(\mathbf{z}))$$

$$\mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0, \quad \mathbf{x}_0 \sim p_0(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$$

Recap of Previous Lecture

Gaussian Conditional Probability Path

$$p_t(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_t(\mathbf{z}), \boldsymbol{\sigma}_t^2(\mathbf{z})) ; \quad \mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0$$

$$\mathbf{f}(\mathbf{x}, \mathbf{z}, t) = \boldsymbol{\mu}'_t(\mathbf{z}) + \frac{\boldsymbol{\sigma}'_t(\mathbf{z})}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{z}))$$

Conditioning Latent Variable

Let's choose $\mathbf{z} = \mathbf{x}_1$. Then $p(\mathbf{z}) = p_1(\mathbf{x}_1)$.

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{x}_1)p_1(\mathbf{x}_1)d\mathbf{x}_1$$

We must ensure the boundary constraints:

$$\begin{cases} p(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_0(\mathbf{x}|\mathbf{z}); (= \mathcal{N}(0, \mathbf{I})) \\ p_{\text{data}}(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_1(\mathbf{x}|\mathbf{z}). \end{cases} \Rightarrow \begin{cases} p_0(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(0, \mathbf{I}); \\ p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases}$$

Recap of Previous Lecture

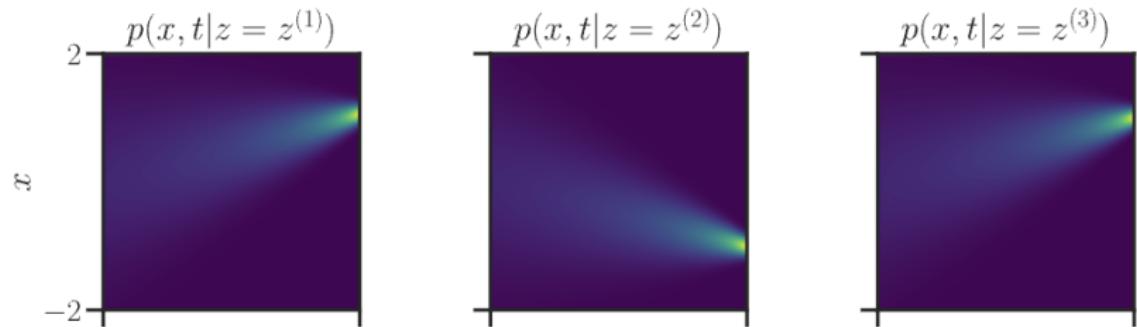
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Gaussian Conditional Probability Path

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Let's consider straight conditional paths:

$$\begin{cases} \boldsymbol{\mu}_t(\mathbf{x}_1) = t\mathbf{x}_1; \\ \boldsymbol{\sigma}_t(\mathbf{x}_1) = 1 - t. \end{cases} \Rightarrow \begin{cases} p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(t\mathbf{x}_1, (1-t)^2\mathbf{I}); \\ \mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0. \end{cases}$$



Recap of Previous Lecture

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(t\mathbf{x}_1, (1-t)^2 \mathbf{I}); \quad \mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0$$

$$\mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}_t}{1-t} = \mathbf{x}_1 - \mathbf{x}_0$$

$$\begin{aligned} & \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \|\mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 = \\ &= \mathbb{E}_{\mathbf{x}_1 \sim p_{\text{data}}(\mathbf{x})} \mathbb{E}_{\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})} \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_\theta(t\mathbf{x}_1 + (1-t)\mathbf{x}_0, t)\|^2 \end{aligned}$$

- ▶ $\mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t)$ defines straight lines between $p_{\text{data}}(\mathbf{x})$ and $\mathcal{N}(0, \mathbf{I})$.
- ▶ The **marginal** path $p_t(\mathbf{x})$ does not give straight lines.



Recap of Previous Lecture

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim p_{\text{data}}(\mathbf{x})} \mathbb{E}_{\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})} \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\theta}(\mathbf{x}_t, t)\|^2 \rightarrow \min_{\theta}$$

Training

1. Sample $\mathbf{x}_1 \sim p_{\text{data}}(\mathbf{x})$.
2. Sample time $t \sim U[0, 1]$ and $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$.
3. Obtain the noisy image $\mathbf{x}_t = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0$.
4. Compute the loss $\mathcal{L} = \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\theta}(\mathbf{x}, t)\|^2$.

Sampling

1. Sample $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$.
2. Solve the ODE to obtain \mathbf{x}_1 :

$$\mathbf{x}_1 = \text{ODESolve}_f(\mathbf{x}_0, \theta, t_0 = 0, t_1 = 1)$$

Recap of Previous Lecture

Let us choose $\mathbf{z} = (\mathbf{x}_0, \mathbf{x}_1)$. Then $p(\mathbf{z}) = p(\mathbf{x}_0, \mathbf{x}_1) = p_0(\mathbf{x}_0)p_1(\mathbf{x}_1)$.

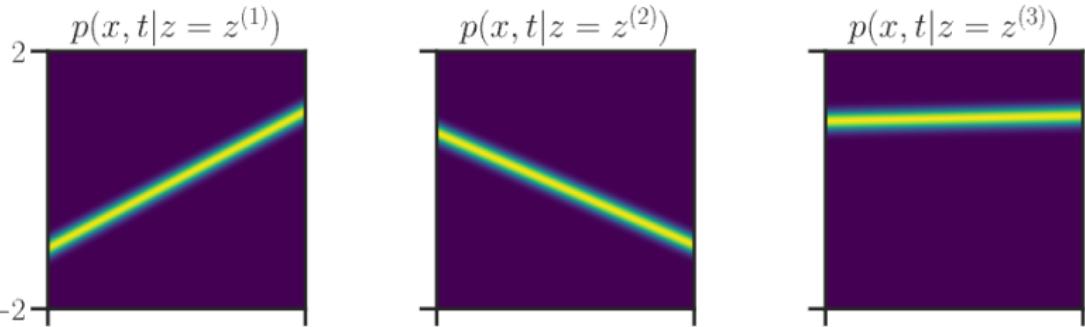
$$p_0(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_0); \quad p_1(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1)$$

Gaussian Conditional Probability Path

$$p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \mathcal{N}(\boldsymbol{\mu}_t(\mathbf{x}_0, \mathbf{x}_1), \boldsymbol{\sigma}_t^2(\mathbf{x}_0, \mathbf{x}_1)); \quad \mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{x}_0, \mathbf{x}_1) + \boldsymbol{\sigma}_t(\mathbf{x}_0, \mathbf{x}_1) \odot \boldsymbol{\epsilon}$$

Let's consider straight conditional paths:

$$\boldsymbol{\mu}_t(\mathbf{x}_1) = t\mathbf{x}_1 + (1-t)\mathbf{x}_0 \quad \boldsymbol{\sigma}_t(\mathbf{x}_1) = \boldsymbol{\epsilon}$$



Recap of Previous Lecture

Endpoint conditioning

$$z = x_1$$

$$p_t(x|x_1) = \mathcal{N}(tx_1, (1-t)^2 I)$$

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

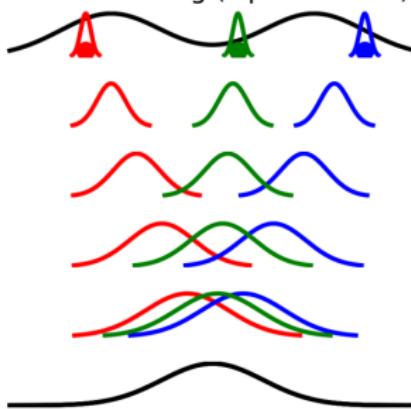
Pair conditioning

$$z = (x_0, x_1)$$

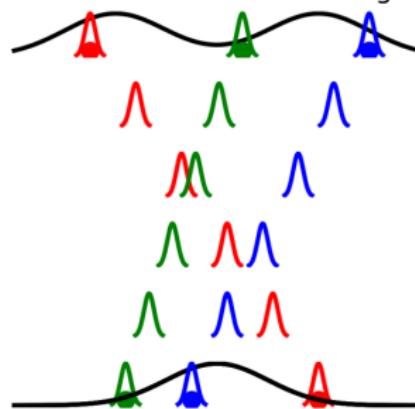
$$p_t(x|x_0, x_1) = \mathcal{N}(tx_1 + (1-t)x_0, \epsilon^2 I)$$

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

Flow Matching (Lipman et al.)



Conditional Flow Matching



Recap of Previous Lecture

- ▶ This conditioning allows us to transport any distribution $p_0(\mathbf{x})$ to any distribution $p_1(\mathbf{x})$.
- ▶ It's possible to apply this approach to paired tasks, e.g., style transfer.

Training Procedure

1. Sample $(\mathbf{x}_0, \mathbf{x}_1) \sim p(\mathbf{x}_0, \mathbf{x}_1)$.
2. Sample time $t \sim U[0, 1]$.
3. Compute the noisy image $\mathbf{x}_t = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0$.
4. Compute the loss $\mathcal{L} = \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\theta}(\mathbf{x}, t)\|^2$.

Sampling

1. Sample $\mathbf{x}_0 \sim p_0(\mathbf{x})$.
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$$\mathbf{x}_1 = \text{ODESolve}_f(\mathbf{x}_0, \theta, t_0 = 0, t_1 = 1)$$

Outline

1. Link between Flow Matching and Score-Based Models
2. Discrete Diffusion Models
 - Forward Discrete Process
 - Reverse Discrete Diffusion

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Score-Based Generative Models through SDEs

Training

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x}(0))} \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{q(\mathbf{x}(t)|\mathbf{x}(0))} \| \mathbf{s}_\theta(\mathbf{x}(t), t) - \nabla_{\mathbf{x}(t)} \log q(\mathbf{x}(t)|\mathbf{x}(0)) \|_2^2$$

Score-Based Generative Models through SDEs

Training

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Variance Exploding SDE (NCSN)

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}(\mathbf{x}(0), [\sigma^2(t) - \sigma^2(0)] \cdot \mathbf{I}), \quad \sigma(0) = 0$$

Variance Preserving SDE (DDPM)

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}(\mathbf{x}(0)\alpha(t), (1 - \alpha(t)^2) \cdot \mathbf{I}); \quad \alpha(t) = e^{-\frac{1}{2} \int_0^t \beta(s) ds}$$

Score-Based Generative Models through SDEs

Training

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x}(0))} \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{q(\mathbf{x}(t)|\mathbf{x}(0))} \| \mathbf{s}_{\theta}(\mathbf{x}(t), t) - \nabla_{\mathbf{x}(t)} \log q(\mathbf{x}(t)|\mathbf{x}(0)) \|_2^2$$

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Flow matching uses reverse time direction:

$$p_t(\mathbf{x}|\mathbf{x}_1) = q_{1-t}(\mathbf{x}|\mathbf{x}_0 = \mathbf{x}_1)$$

Score-Based Generative Models through SDEs

$$p_t(\mathbf{x}_t | \mathbf{x}_1) = q_{1-t}(\mathbf{x}_{1-t} | \mathbf{x}_0 = \mathbf{x}_1)$$

VE (NCSN): $p_t(\mathbf{x} | \mathbf{x}_1) = \mathcal{N}(\mathbf{x}_1, \sigma_{1-t}^2 \cdot \mathbf{I})$

VP (DDPM): $p_t(\mathbf{x} | \mathbf{x}_1) = \mathcal{N}(\alpha_{1-t} \mathbf{x}_1, (1 - \alpha_{1-t}^2) \cdot \mathbf{I})$

Score-Based Generative Models through SDEs

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Flow Matching Probability Path

$$p_t(\mathbf{x} | \mathbf{x}_1) = \mathcal{N}(t\mathbf{x}_1, (1 - t)^2 \mathbf{I}) ; \quad \mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}_t}{1 - t}$$

$$\frac{d\mathbf{x}_t}{dt} = \mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = \mu'_t(\mathbf{x}_1) + \frac{\sigma'_t(\mathbf{x}_1)}{\sigma_t(\mathbf{x}_1)} \odot (\mathbf{x}_t - \mu_t(\mathbf{x}_1))$$

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Let's derive the conditional vector fields for VE (NCSN) and VP (DDPM).

Flow Matching vs. Score-Based SDE Models

$$\frac{d\mathbf{x}_t}{dt} = \mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = \boldsymbol{\mu}'_t(\mathbf{x}_1) + \frac{\boldsymbol{\sigma}'_t(\mathbf{x}_1)}{\boldsymbol{\sigma}_t(\mathbf{x}_1)} \odot (\mathbf{x}_t - \boldsymbol{\mu}_t(\mathbf{x}_1))$$

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Variance Exploding SDE Probability Path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\mathbf{x}_1, \sigma_{1-t}^2 \mathbf{I}) \quad \Rightarrow \quad \mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = -\frac{\sigma'_{1-t}}{\sigma_{1-t}}(\mathbf{x}_t - \mathbf{x}_1)$$

Flow Matching vs. Score-Based SDE Models

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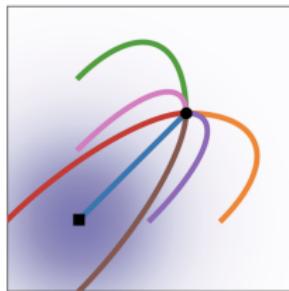
Variance Preserving SDE Probability Path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\alpha_{1-t}\mathbf{x}_1, (1 - \alpha_{1-t}^2)\mathbf{I}) \Rightarrow \mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = \frac{\alpha'_{1-t}}{1 - \alpha_{1-t}^2} \cdot (\alpha_{1-t}\mathbf{x}_t - \mathbf{x}_1)$$

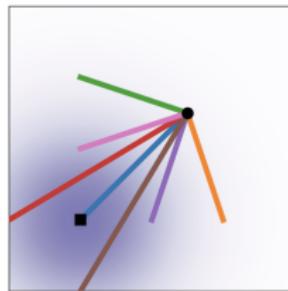
Thus, VE/VP SDE models correspond to particular choices of the Gaussian probability path within the flow matching framework.

Flow Matching vs. Score-Based SDE Models

Trajectories



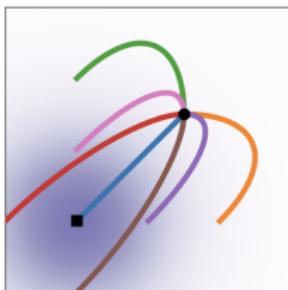
Diffusion



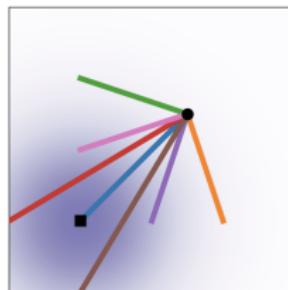
OT

Flow Matching vs. Score-Based SDE Models

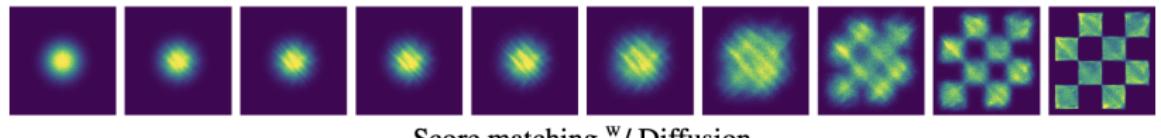
Trajectories



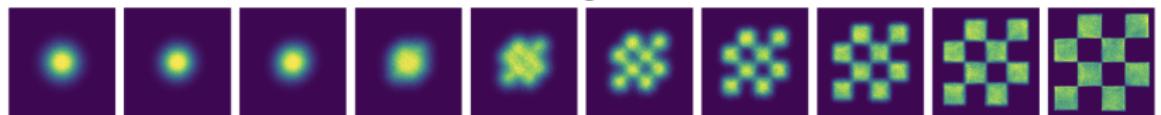
Diffusion



OT



Score matching w/ Diffusion



Flow Matching w/ OT

Outline

1. Link between Flow Matching and Score-Based Models
2. Discrete Diffusion Models
 - Forward Discrete Process
 - Reverse Discrete Diffusion

Discrete or Continuous Diffusion Models?

Reminder: Diffusion models define a forward corruption process and a reverse denoising process. Previously, we studied diffusion models with continuous states $\mathbf{x}(t) \in \mathbb{R}^m$.

Continuous state space

- ▶ **Discrete time** $t \in \{0, 1, \dots, T\} \Rightarrow \text{DDPM / NCSN.}$
- ▶ **Continuous time** $t \in [0, 1] \Rightarrow \text{Score-based SDE models.}$

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- ▶ **Continuous time** $t \in [0, 1] \Rightarrow \text{Score-based SDE models.}$

Now we turn to diffusion over discrete-value states
 $\mathbf{x}(t) \in \{1, \dots, K\}^m$.

Discrete state space

- ▶ **Discrete time** $t \in \{0, 1, \dots, T\}.$
- ▶ **Continuous time** $t \in [0, 1].$

Let's discuss why we need discrete diffusion models.

Why Discrete Diffusion Models?

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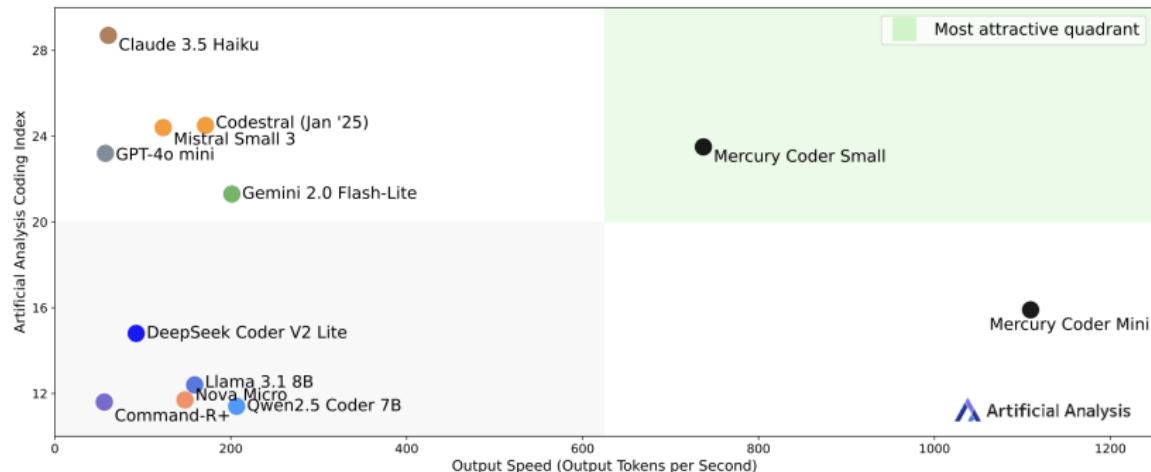
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- ▶ **Robustness:** diffusion avoids the "exposure bias" caused by teacher forcing in AR training.
- ▶ **Unified framework:** diffusion generalizes naturally to discrete domains that do not suit continuous Gaussian noise.

2025 – Big Bang of Discrete Diffusion Models

Coding Index vs. Output Speed: Smaller models

Artificial Analysis Coding Index (represents the average of LiveCodeBench & SciCode);
Output Speed: Output Tokens per Second; 1,000 Input Tokens; Coding focused workload



Outline

1. Link between Flow Matching and Score-Based Models

2. Discrete Diffusion Models

Forward Discrete Process

Reverse Discrete Diffusion

Forward Discrete Process

Continuous Diffusion Markov Chain

In continuous diffusion, the forward Markov chain is defined by progressively corrupting data with Gaussian noise:

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I}).$$

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Discrete Diffusion Markov Chain

For discrete data, we instead define a Markov chain over categorical states:

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$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \text{Cat}(\mathbf{Q}_t \mathbf{x}_{t-1}),$$

- ▶ Each $\mathbf{x}_t \in \{0, 1\}^K$ is a **one-hot vector** encoding the categorical state (it is just one token).
- ▶ What is the transition matrix \mathbf{Q}_t ?

Forward Process over Time

Transition Matrix

$\mathbf{Q}_t \in [0, 1]^{K \times K}$ is a **transition matrix** where each column gives transition probabilities from one state to all others, and columns sum to 1:

$$[\mathbf{Q}_t]_{ij} = q(x_t = i | x_{t-1} = j), \quad \sum_{i=1}^K [\mathbf{Q}_t]_{ij} = 1.$$

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- ▶ The forward diffusion gradually destroys information through repeated random transitions.

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$$[\mathbf{Q}_t]_{ij} = q(x_t = i | x_{t-1} = j), \quad \sum_{i=1}^K [\mathbf{Q}_t]_{ij} = 1.$$

- ▶ The forward diffusion gradually destroys information through repeated random transitions.
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Forward Process over Time

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- ▶ As $t \rightarrow T$, the process drives the data toward a stationary distribution.
- ▶ We design the transition matrices \mathbf{Q}_t to achieve this behavior.

Transition Matrix

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Common choices

- ▶ **Uniform diffusion**

$$\mathbf{Q}_t = (1 - \beta_t)\mathbf{I} + \beta_t\mathbf{U}, \quad \mathbf{U}_{ij} = \frac{1}{K}.$$

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- ▶ **Absorbing diffusion**

$$\mathbf{Q}_t = (1 - \beta_t)\mathbf{I} + \beta_t \mathbf{e}_m \mathbf{1}^\top.$$

Tokens are gradually replaced by a special mask m ; the stationary distribution is fully masked.

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$$q(\mathbf{x}_t | \mathbf{x}_0) = \text{Cat}(\mathbf{Q}_{1:t} \mathbf{x}_0), \quad \mathbf{Q}_{1:t} = \mathbf{Q}_t \mathbf{Q}_{t-1} \cdots \mathbf{Q}_1.$$

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- ▶ Each token retains its original value with prob. $\bar{\alpha}_t$.
- ▶ It becomes uniformly random with prob. $(1 - \bar{\alpha}_t)$.
- ▶ As $t \rightarrow T$, the process converges to the stationary uniform distribution.

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- ▶ Each token retains its original value with prob. $\bar{\alpha}_t$.
- ▶ It becomes \mathbf{e}_m with prob. $(1 - \bar{\alpha}_t)$.
- ▶ As $t \rightarrow T$, all tokens converge to the mask state:
 $q(\mathbf{x}_T) \approx \text{Cat}(\mathbf{e}_m)$.
- ▶ This makes the process analogous to **masked language modeling**.

Uniform vs. Absorbing Transition Matrix

Aspect	Uniform Diffusion	Absorbing Diffusion
\mathbf{Q}_t	$(1 - \beta_t)\mathbf{I} + \beta_t\mathbf{U}$	$(1 - \beta_t)\mathbf{I} + \beta_t\mathbf{e}_m\mathbf{1}^\top$
$\mathbf{Q}_{1:t}$	$\bar{\alpha}_t\mathbf{I} + (1 - \bar{\alpha}_t)\mathbf{U}$	$\bar{\alpha}_t\mathbf{I} + (1 - \bar{\alpha}_t)\mathbf{e}_m\mathbf{1}^\top$
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Observation

Both schemes gradually destroy information, but differ in their stationary limit. Absorbing diffusion bridges diffusion and masked-language-model objectives.

Outline

1. Link between Flow Matching and Score-Based Models

2. Discrete Diffusion Models

Forward Discrete Process

Reverse Discrete Diffusion

Posterior of the Forward Process

ELBO

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) = & \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ & - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{\mathcal{L}_t}\end{aligned}$$

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- ▶ Conditioned reverse distribution $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ played crucial role in the continuous-state diffusion model.
- ▶ It shows the probability of a previous state given the noisy state \mathbf{x}_t and the original clean data \mathbf{x}_0 .

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Discrete conditioned reverse distribution

$$\begin{aligned}q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0) q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} \\ &= \frac{\text{Cat}(\mathbf{Q}_t) \cdot \text{Cat}(\mathbf{Q}_{1:t-1})}{\text{Cat}(\mathbf{Q}_{1:t})}.\end{aligned}$$

Posterior of the Forward Process

Discrete conditioned reverse distribution

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) = \text{Cat} \left(\frac{\mathbf{Q}_t \mathbf{x}_t \odot \mathbf{Q}_{1:t-1} \mathbf{x}_0}{\mathbf{x}_t^\top \mathbf{Q}_{1:t} \mathbf{x}_0} \right).$$

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Recall the ELBO term

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) \| p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)),$$

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- ▶ Both $q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0)$ and $q(\mathbf{x}_t | \mathbf{x}_0)$ are known analytically from the forward process.
- ▶ The reverse process $p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$ is a learned categorical distribution:

$$p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) = \text{Cat}(\pi_\theta(\mathbf{x}_t, t)),$$

where π_θ is a neural network.

Discrete-time ELBO for Discrete Diffusion

ELBO term

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}\left(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)\right).$$

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Categorical KL

$$\text{KL}(\text{Cat}(\mathbf{q}) \parallel \text{Cat}(\mathbf{p})) = \sum_{k=1}^K q_k \log \frac{q_k}{p_k} = H(\mathbf{q}, \mathbf{p}) - H(\mathbf{q}),$$

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- ▶ $H(\mathbf{q}, \mathbf{p}) = -\sum_k q_k \log p_k$ is a **cross-entropy loss**.

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- ▶ $H(\mathbf{q}, \mathbf{p}) = -\sum_k q_k \log p_k$ is a **cross-entropy loss**.

Therefore, minimizing \mathcal{L}_t w.r.t. θ is equivalent to minimizing

$$\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} H(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0), p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)).$$

Summary

- ▶ Diffusion and score-based models are special cases of the flow matching approach, but use curved trajectories.
- ▶ Diffusion approach has several key advantages over autoregressive approach.
- ▶ Forward discrete diffusion process defines Markov chain with discrete states.
- ▶ There are several ways to make it tractable (uniform / absorbing transitions).
- ▶ Reverse discrete diffusion process uses the variational approach to invert forward process.
- ▶ Discrete-state ELBO for discrete diffusion is a cross-entropy loss.