Deep Generative Models

Lecture 13

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2025, Autumn

Recap of Previous Lecture

Flow Matching (FM)

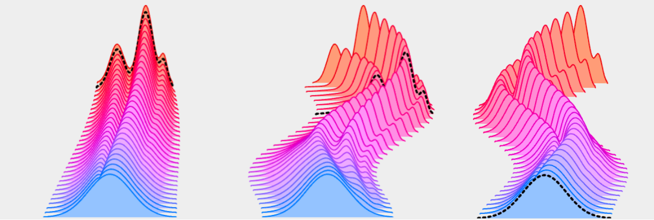
$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \left\| \mathbf{f}(\mathbf{x}, t) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \to \min_{\boldsymbol{\theta}}$$

Conditional Flow Matching (CFM)

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

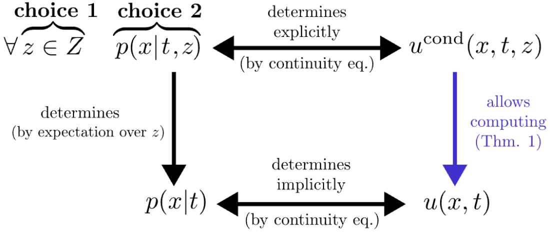
Theorem

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



Tong A., et al. Improving and Generalizing Flow-Based Generative Models with Minibatch Optimal Transport, 2023

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

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

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

image credit: A Visual Dive into Conditional Flow Matching

Recap of Previous Lecture

Gaussian Conditional Probability Path

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

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:

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

Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Recap of Previous Lecture

$$p_0(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(0, \mathbf{I}); \quad p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1).$$

Gaussian Conditional Probability Path

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

Let's consider straight conditional paths:

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

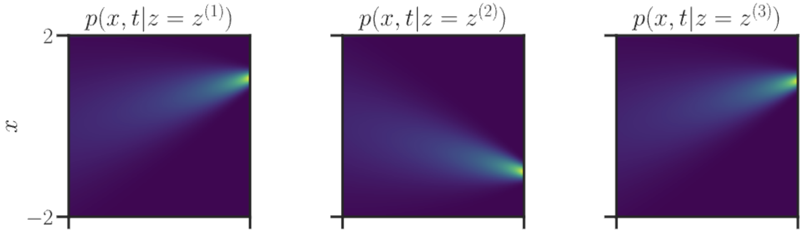

image credit: A Visual Dive into Conditional Flow Matching

Recap of Previous Lecture

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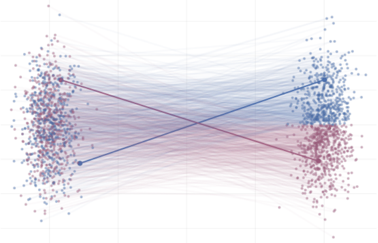
$$\mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}_t}{1-t} = \mathbf{x}_1 - \mathbf{x}_0$$

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

- $\mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t)$ 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.



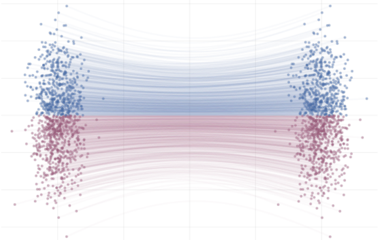


image credit: https://mlg.eng.cam.ac.uk/blog/2024/01/20/flow-matching.html

Recap of Previous Lecture

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

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 $\mathcal{L} = \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t)\|^2$.

Sampling

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

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

Lipman Y., et al. Flow Matching for Generative Modeling, 2022

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

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

Let's consider straight conditional paths:

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

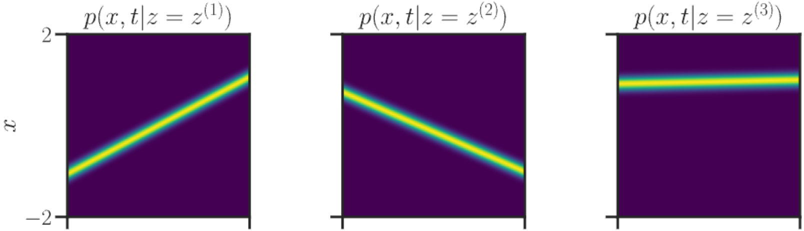


image credit: A Visual Dive into Conditional Flow Matching

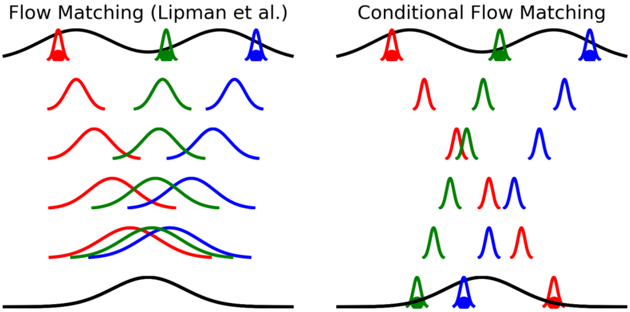
Recap of Previous Lecture

Endpoint conditioning

$$
\begin{aligned}
\mathbf{z} &= \mathbf{x}_1 \\
p_t(\mathbf{x}|\mathbf{x}_1) &= \mathcal{N}\left(t\mathbf{x}_1, (1-t)^2\mathbf{I}\right) \\
\mathbf{x}_t &= t\mathbf{x}_1 + (1-t)\mathbf{x}_0
\end{aligned}
$$

Pair conditioning

$$
\begin{aligned}
\mathbf{z} &= (\mathbf{x}_0, \mathbf{x}_1) \\
p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) &= \mathcal{N}\left(t\mathbf{x}_1 + (1-t)\mathbf{x}_0, \epsilon^2\mathbf{I}\right) \\
\mathbf{x}_t &= t\mathbf{x}_1 + (1-t)\mathbf{x}_0
\end{aligned}
$$



Tong A., et al. Improving and Generalizing Flow-Based Generative Models with Minibatch Optimal Transport, 2023

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 $\mathbf{x}_t = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0$.
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Sampling

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Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Recap of Previous Lecture

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

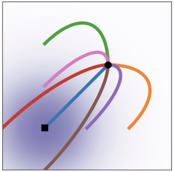
$$p_t(\mathbf{x}_t|\mathbf{x}_1) = q_{1-t}(\mathbf{x}_{1-t}|\mathbf{x}_0 = \mathbf{x}_1)$$

Variance Exploding SDE

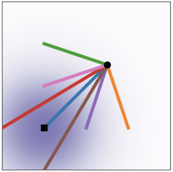
$$p_t(\mathbf{x}_t|\mathbf{x}_1) = \mathcal{N}\left(\mathbf{x}_1, \sigma_{1-t}^2\mathbf{I}\right) \quad \Rightarrow \quad \mathbf{f}(\mathbf{x}_t, \mathbf{x}_1, t) = -\frac{\sigma'_{1-t}}{\sigma_{1-t}}(\mathbf{x}_t - \mathbf{x}_1)$$

Variance Preserving SDE

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



Diffusion



OT

Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Outline

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

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

Discrete state space

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

Let's discuss why we need discrete diffusion models.

Why Discrete Diffusion Models?

While autoregressive (AR) models dominate discrete-data domains (e.g., text or sequences), they have fundamental limitations.

https://aaronlou.com/blog/2024/discrete-diffusion/

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Key advantages of discrete diffusion

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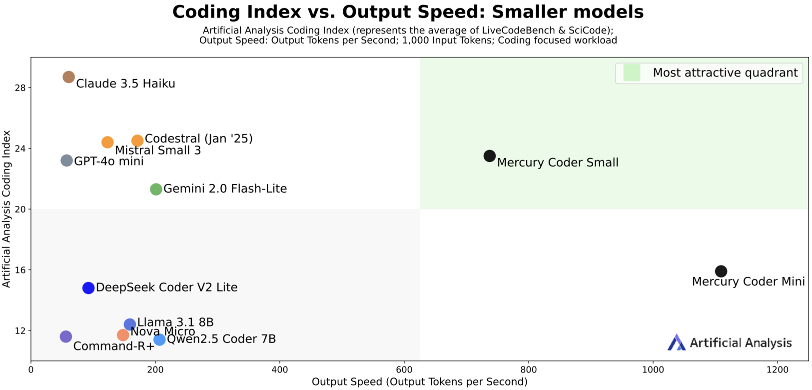
- **Robustness:** diffusion avoids the "exposure bias" caused by teacher forcing in AR training.
- **Unified framework:** diffusion generalizes naturally to discrete domains that do not suit continuous Gaussian noise.

https://aaronlou.com/blog/2024/discrete-diffusion/

2025 – Big Bang of Discrete Diffusion Models



Khanna S. et al. Mercury: Ultra-fast language models based on diffusion, 2025.

Outline

Forward Discrete Process

Continuous Diffusion Markov Chain

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

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

Austin J. et al. Structured denoising diffusion models in discrete state-spaces, 2021.

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Discrete Diffusion Markov Chain

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

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

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

- 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 $\mathbf{Q}_t$?

Austin J. et al. Structured denoising diffusion models in discrete state-spaces, 2021.

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:

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

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- Applying the transition t times yields the marginal distribution:

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

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- As $t \to T$, the process drives the data toward a stationary distribution.

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

Austin J. et al. Structured denoising diffusion models in discrete state-spaces, 2021.

Transition Matrix

- The choice of $\mathbf{Q}_t$ determines how information is erased and what the stationary distribution becomes.

Austin J. et al. Structured denoising diffusion models in discrete state-spaces, 2021.

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Austin J. et al. Structured denoising diffusion models in discrete state-spaces, 2021.

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Common choices

- **Uniform diffusion**

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

Each token is replaced by a uniformly random symbol with probability β_t. The stationary distribution is uniform noise.

Austin J. et al. Structured denoising diffusion models in discrete state-spaces, 2021.

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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.

Austin J. et al. Structured denoising diffusion models in discrete state-spaces, 2021.

Transition Matrix

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

Transition Matrix

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Uniform Diffusion

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

$$\mathbf{Q}_{1:t} = \bar{\alpha}_t\mathbf{I} + (1-\bar{\alpha}_t)\mathbf{U}, \quad \bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s).$$

Transition Matrix

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

Uniform Diffusion

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$$\mathbf{Q}_{1:t} = \bar{\alpha}_t\mathbf{I} + (1-\bar{\alpha}_t)\mathbf{U}, \quad \bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s).$$

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

Transition Matrix

Absorbing Diffusion

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

$$\mathbf{Q}_{1:t} = \bar{\alpha}_t \, \mathbf{I} + (1 - \bar{\alpha}_t) \, \mathbf{e}_m \mathbf{1}^\top, \qquad \bar{\alpha}_t = \prod_{s=1}^{t} (1 - \beta_s).$$

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

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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 $t \to T$, all tokens converge to the mask state: $q(\mathbf{x}_T) \approx \mathrm{Cat}(\mathbf{e}_m)$.
- This makes the process analogous to **masked language modeling**.

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Uniform vs. Absorbing Transition Matrix

Aspect	**Uniform Diffusion**	**Absorbing Diffusion**
$\mathbf{Q}_t$	$(1-\beta_t)\mathbf{I}+\beta_t\mathbf{U}$	$(1-\beta_t)\mathbf{I}+\beta_t\mathbf{e}_m\mathbf{1}^\top$
$\mathbf{Q}_{1:t}$	$\bar{\alpha}_t\mathbf{I}+(1-\bar{\alpha}_t)\mathbf{U}$	$\bar{\alpha}_t\mathbf{I}+(1-\bar{\alpha}_t)\mathbf{e}_m\mathbf{1}^\top$
$\mathbf{Q}_{1:\infty}$	$\mathbf{U}$	$\mathrm{Cat}(\mathbf{e}_m)$
Interpretation	Random replacement	Gradual masking of tokens
Application	Image / symbol diffusion	Text diffusion $\approx$ Masked LM

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Uniform vs. Absorbing Transition Matrix

Aspect	Uniform Diffusion	Absorbing Diffusion
$\mathbf{Q}_t$	$(1-\beta_t)\mathbf{I} + \beta_t \mathbf{U}$	$(1-\beta_t)\mathbf{I} + \beta_t \mathbf{e}_m \mathbf{1}^\top$
$\mathbf{Q}_{1:t}$	$\bar{\alpha}_t \mathbf{I} + (1-\bar{\alpha}_t)\mathbf{U}$	$\bar{\alpha}_t \mathbf{I} + (1-\bar{\alpha}_t)\mathbf{e}_m \mathbf{1}^\top$
$\mathbf{Q}_{1:\infty}$	$\mathbf{U}$	$\mathrm{Cat}(\mathbf{e}_m)$
Interpretation	Random replacement	Gradual masking of tokens
Application	Image / symbol diffusion	Text diffusion $\approx$ Masked LM

Observation

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

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Outline

Posterior of the Forward Process

ELBO

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

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

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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 $\mathbf{x}_0$.

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

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Discrete conditioned reverse distribution

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

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Posterior of the Forward Process

Discrete conditioned reverse distribution

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

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Posterior of the Forward Process

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Recall the ELBO term

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

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Discrete conditioned reverse distribution

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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 $p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is a learned categorical distribution:

$$p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathrm{Cat}\big(\boldsymbol{\pi}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)\big),$$

where $\boldsymbol{\pi}_{\boldsymbol{\theta}}$ is a neural network.

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Discrete-time ELBO for Discrete Diffusion

ELBO term

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

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

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Categorical KL

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

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

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

- $\mathrm{H}\big(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\big)$ is a constant w.r.t. $\boldsymbol{\theta}$.
- $\mathrm{H}(\mathbf{q}, \mathbf{p}) = -\sum_k q_k \log p_k$ is a **cross-entropy loss**.

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

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

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

- $\mathrm{H}\big(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\big)$ is a constant w.r.t. $\boldsymbol{\theta}$.
- $\mathrm{H}(\mathbf{q}, \mathbf{p}) = -\sum_k q_k \log p_k$ is a **cross-entropy loss**.

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

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

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Outline

Absorbing Diffusion: Forward Process

Let's restrict to the case of absorbing transition matrix. At each step t:

- with probability $(1 - \beta_t)$ a token is kept;
- with probability β_t it is replaced by the mask token m.

$$\mathbf{Q}_t = (1 - \beta_t)\mathbf{I} + \beta_t\,\mathbf{e}_m \mathbf{1}^\top, \qquad \bar{\alpha}_t = \prod_{s=1}^{t}(1 - \beta_s).$$

$$\mathbf{Q}_{1:t} = \bar{\alpha}_t\,\mathbf{I} + (1 - \bar{\alpha}_t)\,\mathbf{e}_m \mathbf{1}^\top.$$

Each position is either still clean or already masked:

$$q(\mathbf{x}_t|\mathbf{x}_0) = \begin{cases} \bar{\alpha}_t, & \mathbf{x}_t = \mathbf{x}_0 \\ 1 - \bar{\alpha}_t, & \mathbf{x}_t = \mathbf{e}_m \\ 0, & \text{otherwise.} \end{cases}$$

Sahoo S. et al. Simple and Effective Masked Diffusion Language Models, 2024

NOT READY

Absorbing / Masked Diffusion: Sequence View

Consider a sequence $\mathbf{x}_0 = (x_0^1, \ldots, x_0^L)$.

Independent masking across positions

Because the forward chain factorizes over positions,

$$q(\mathbf{x}_t \mid \mathbf{x}_0) = \prod_{\ell=1}^{L} q(x_t^\ell \mid x_0^\ell),$$

and for each position ℓ:

$$q(x_t^\ell = x_0^\ell \mid \mathbf{x}_0) = \bar{\alpha}_t, \qquad q(x_t^\ell = m \mid \mathbf{x}_0) = 1 - \bar{\alpha}_t.$$

- At small t, most tokens remain clean; a few are masked.
- As $t \to T$, almost all tokens become m and $q(\mathbf{x}_T)$ is concentrated on the fully masked sequence.
- This gives a **multi-step masking schedule**, instead of BERT's single-step masking.

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Posterior in Absorbing Diffusion: Unmask vs Stay Masked

Recall the general discrete posterior

$$q(x_{t-1} \mid x_t, x_0) = \frac{q(x_t \mid x_{t-1})\, q(x_{t-1} \mid x_0)}{q(x_t \mid x_0)}.$$

For the absorbing process we can obtain a closed-form expression.

Case 1: $x_t = x_0$ (token not yet masked)

Because the mask is absorbing, we cannot go from mask back to a clean token:

$$q(x_{t-1} = x_0 \mid x_t = x_0, x_0) = 1.$$

If we observe $x_t = x_0$, we know the token has **never been masked** up to time t.

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Posterior in Absorbing Diffusion: Unmask vs Stay Masked

Case 2: $x_t = m$ (token is masked)

Now x_{t-1} could be:

- already masked at $t-1$ and stayed masked, or
- still clean (x_0) at $t-1$ and masked only at step t.

Using the forward marginals,

$$q(x_{t-1} = x_0 \mid x_t = m, x_0) = \frac{\bar{\alpha}_{t-1}\,\beta_t}{1-\bar{\alpha}_t},$$

$$q(x_{t-1} = m \mid x_t = m, x_0) = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t},$$

and all other states have probability 0.

Posterior in Absorbing Diffusion: Interpretation

Unmask vs stay masked

When $x_t = m$,

$$q(x_{t-1} \mid x_t = m, x_0) = \underbrace{\frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t}}_{\text{already masked}} \; \delta_{x_{t-1}=m} + \underbrace{\frac{\bar{\alpha}_{t-1}\beta_t}{1 - \bar{\alpha}_t}}_{\text{just masked}} \; \delta_{x_{t-1}=x_0}.$$

- The posterior is a simple binary choice:
  - **stay masked**: keep $x_{t-1} = m$,
  - **unmask**: revert to the original symbol x_0.
- The reverse model $p_{\boldsymbol{\theta}}(x_{t-1} \mid x_t)$ learns, at masked positions, how likely it is to *unmask* vs *stay masked*.
- This is exactly the semantic of **iterative infilling**: tokens start from mask and are gradually turned into meaningful symbols.

ELBO Term for Absorbing Diffusion

Recall the per-timestep ELBO term

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

Categorical KL $\Rightarrow$ cross-entropy

As before,

$$\mathrm{KL}\big(\mathrm{Cat}(\mathbf{q}) \,\|\, \mathrm{Cat}(\mathbf{p})\big) = \mathrm{H}(\mathbf{q}, \mathbf{p}) - \mathrm{H}(\mathbf{q}),$$

and the entropy term $\mathrm{H}(\mathbf{q})$ does not depend on $\boldsymbol{\theta}$.
Therefore minimizing $\mathcal{L}_t$ is equivalent (w.r.t. $\boldsymbol{\theta}$) to

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

- For absorbing diffusion, $q(x_{t-1}^\ell \mid x_t^\ell, x_0^\ell)$ is supported only on $\{x_0^\ell, m\}$.
- This makes the target distribution extremely simple, and opens the door to a much simpler training loss.

Austin J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.

Simplified Training: Predict Clean Token at Masked Positions

Key observation

For absorbing diffusion:

- If $x_t^\ell \neq m$, then $x_t^\ell = x_0^\ell$ and the posterior $q(x_{t-1}^\ell \mid x_t^\ell, x_0^\ell)$ is a delta at x_0^ℓ.
- If $x_t^\ell = m$, the posterior is a binary distribution over $\{m, x_0^\ell\}$.

The informative supervision is concentrated at **masked positions**.

Austin, J. et al., Structured denoising diffusion models in discrete state-spaces, 2021.
See also recent refinements in arXiv:2406.07524.

Simplified Training: Predict Clean Token at Masked Positions

Practical training objective

In practice we parameterize the model to predict x_0 from $(\mathbf{x}_t, t)$:

$$p_{\boldsymbol{\theta}}(x_0^\ell \mid \mathbf{x}_t, t) = \mathrm{Cat}\big(\boldsymbol{\pi}_\theta(\mathbf{x}_t, t)^\ell\big),$$

and minimize a time-conditioned cross-entropy:

$$\mathcal{L}_{\text{mask}}(\theta) = \mathbb{E}_{t,\, \mathbf{x}_0,\, \mathbf{x}_t \sim q(\mathbf{x}_t \mid \mathbf{x}_0)} \sum_{\ell=1}^{L} w_t \, \mathbb{I}\{x_t^\ell = m\} \big[-\log p_{\boldsymbol{\theta}}(x_0^\ell \mid \mathbf{x}_t, t)\big].$$

- w_t – optional weighting over timesteps (e.g., uniform over t).
- We apply cross-entropy only at positions where the input token is masked.

Absorbing Diffusion as Multi-step Masked LM

- Forward process: gradually replace tokens by a mask m according to a diffusion schedule $\{\beta_t\}$.
- Reverse process: starting from an all-mask sequence, iteratively **unmask** positions by predicting clean tokens x_0 from $(\mathbf{x}_t, t)$.
- Training: time-conditioned masked language modeling objective on masked positions:

$$(\mathbf{x}_0, t) \;\mapsto\; \mathbf{x}_t \sim q(\mathbf{x}_t \mid \mathbf{x}_0), \quad \text{predict } x_0^\ell \text{ wherever } x_t^\ell = m.$$

- This perspective makes absorbing diffusion feel very close to BERT-style masked LMs, but with:
  - a **multi-step** corruption schedule,
  - explicit modeling of the full reverse Markov chain.

Summary