Deep Generative Models

Lecture 14

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Recap of Previous Lecture

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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- **Flexible infilling:**. diffusion can mask arbitrary parts of a sequence and reconstruct them, rather than generating only from prefix to suffix.
- **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.

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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:

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

where $\mathbf{Q}_t \in [0,1]^{K\times K}$ 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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- We design the transition matrices $\mathbf{Q}_t$ to achieve this behavior.

Transition Matrix

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- $\mathbf{Q}_t$ and $\mathbf{Q}_{1:t}$ should be easy to compute for each t.
- **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.

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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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- 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

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

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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.

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

NOT READY

Reverse Process and Model Parameterization

Goal

Learn a reverse model that reconstructs cleaner data from corrupted inputs:

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

Austin J. et al., 2021.

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- The reverse chain defines the generative process:

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- We parameterize $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ as a factorized categorical distribution:

$$p_\theta(x_{t-1,i}|x_t) = \mathrm{Categorical}(x_{t-1,i}; \pi_\theta(x_t, i, t)),$$

where π_θ are model logits over K symbols.

Austin J. et al., 2021.

Variational Objective (Discrete ELBO)

Evidence Lower Bound

$$\log p_\theta(\mathbf{x}_0) \geq \mathbb{E}_q\Big[\sum_{t=1}^{T} -D_{\mathrm{KL}}\big(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)\big)\Big].$$

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For categorical transitions, the KL becomes a cross-entropy term:

$$\mathcal{L}_t = \mathbb{E}_{\mathbf{x}_0, t}[-\log p_\theta(x_{t-1} = x_0 \mid \mathbf{x}_t, t)].$$

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$$\mathcal{L}_t = \mathbb{E}_{\mathbf{x}_0,t}[-\log p_\theta(x_{t-1}{=}x_0 \mid \mathbf{x}_t, t)].$$

- Equivalent to predicting the clean token x_0 from a partially noised $\mathbf{x}_t$.
- In practice, the model learns to *denoise* corrupted inputs at multiple noise levels.

Austin J. et al., 2021.

Relation to Masked Language Modeling (MLM)

- In absorbing diffusion, corrupted tokens are replaced by a mask m.
- The denoising task becomes identical to predicting masked tokens:

$$\mathcal{L} = \mathbb{E}_{t \sim p(t)} \mathbb{E}_{\mathbf{x}_t \sim q(\mathbf{x}_t | \mathbf{x}_0)} [-\log p_\theta(\mathbf{x}_0 | \mathbf{x}_t, t)].$$

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- Therefore, discrete diffusion can be seen as a **mixture of MLM objectives** with varying masking rates.
- This view directly connects diffusion LMs to BERT-style training, but provides a principled probabilistic framework.

Austin J. et al., 2021.

Summary