

Deep Generative Models

Lecture 14

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AI Masters

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Recap of Previous Lecture

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

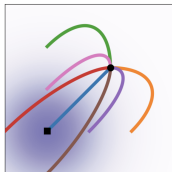
$$p_t(\mathbf{x}|\mathbf{x}_1) = q_{1-t}(\mathbf{x}|\mathbf{x}_0 = \mathbf{x}_1)$$

Variance Exploding SDE

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

Variance Preserving SDE

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



Diffusion



OT

Recap of Previous Lecture

Continuous state space

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

Discrete state space

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

Key advantages of discrete diffusion

- ▶ Parallel generation
- ▶ Flexible infilling
- ▶ Robustness
- ▶ Unified framework

Recap of Previous Lecture

Discrete Diffusion Markov Chain

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

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

Transition Matrix

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

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

- ▶ The choice of \mathbf{Q}_t determines how information is erased and what the stationary distribution becomes.
- ▶ \mathbf{Q}_t and $\mathbf{Q}_{1:t}$ should be easy to compute for each t .

Recap of Previous Lecture

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}	$\text{Cat}(\mathbf{e}_m)$
Interpretation	Random replacement	Gradual masking of tokens
Application	Image 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.

Recap of Previous Lecture

ELBO

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

Discrete conditioned reverse distribution

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

- ▶ 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:

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

Recap of Previous Lecture

ELBO term

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

Categorical KL

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

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

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

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

Outline

1. Discrete Diffusion

From Token to Sequence

Absorbing Diffusion

Continuous-Time Formulation

2. Course Overview

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From Token to Sequence

One-hot sequence representation

$$\mathbf{x}_t \in \{0, 1\}^K \quad \Leftrightarrow \quad \mathbf{X}_t \in \{0, 1\}^{K \times m}$$

Here \mathbf{X}_t is a one-hot representation of a sequence of tokens.

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Independent Token-wise Forward Process

$$q(\mathbf{X}_t | \mathbf{X}_{t-1}) = \prod_{i=1}^m q(\mathbf{x}_t^i | \mathbf{x}_{t-1}^i) = \text{Cat}(\mathbf{Q}_t \mathbf{X}_{t-1})$$

- ▶ Each position i evolves according to its own Markov chain.
- ▶ Often the same transition matrix \mathbf{Q}_t is shared across i .

From Token to Sequence

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Continuous Diffusion Analogy

- ▶ In Gaussian DDPMs with diagonal covariance, noise is independent per pixel.
- ▶ Structure is not in the noise; it is learned by the reverse model.

From Token to Sequence

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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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- ▶ All distributions defined by the forward process are factorized.
- ▶ Dependence appears in the learned reverse model.

Reverse Model for Sequence

$$p_{\theta}(\mathbf{X}_{t-1}|\mathbf{X}_t) = \prod_{i=1}^m p_{\theta}(\mathbf{x}_{t-1}^i|\mathbf{X}_t).$$

- ▶ The output factorizes (parallel prediction across positions).
- ▶ Each factor conditions on the entire noisy sequence \mathbf{X}_t .
- ▶ This is exactly the **masked language modeling** pattern.

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Objective: \mathcal{L}_t term

$$\begin{aligned} \text{KL}(q(\mathbf{X}_{t-1}|\mathbf{X}_t, \mathbf{X}_0) \parallel p_{\theta}(\mathbf{X}_{t-1}|\mathbf{X}_t)) \\ = \sum_{i=1}^m \text{KL}(q(\mathbf{x}_{t-1}^i|\mathbf{x}_t^i, \mathbf{x}_0^i) \parallel p_{\theta}(\mathbf{x}_{t-1}^i|\mathbf{X}_t)). \end{aligned}$$

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Final objective: masked LM

$$\mathcal{L} = \sum_{t=1}^T \sum_{i=1}^m \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[-\log p_{\theta}(\mathbf{x}_0^i|\mathbf{X}_t) \right].$$

Outline

1. Discrete Diffusion

From Token to Sequence

Absorbing Diffusion

Continuous-Time Formulation

2. Course Overview

Absorbing Diffusion: Forward Process

Let's restrict to the case of absorbing transition matrix.

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

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

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Each position is either still clean or already masked:

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$$\mathbf{Q}_t = \begin{pmatrix} 1 - \beta_t & 0 & 0 \\ 0 & 1 - \beta_t & 0 \\ \beta_t & \beta_t & 1 \end{pmatrix} \Rightarrow \text{the masked state is absorbing.}$$

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What happens in the conditioned reverse process $q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0)$?

Absorbing Diffusion

Conditioned reverse distribution

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \begin{cases} [\mathbf{x}_{t-1} = \mathbf{x}_t], & \text{if } \mathbf{x}_t \neq \mathbf{e}_m, \\ \rho_t[\mathbf{x}_{t-1} = \mathbf{x}_0] + (1 - \rho_t)[\mathbf{x}_{t-1} = \mathbf{e}_m], & \text{if } \mathbf{x}_t = \mathbf{e}_m, \end{cases}$$

where

$$\rho_t = \frac{\beta_t \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t}.$$

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- ▶ If $\mathbf{x}_t \neq \mathbf{e}_m$, then the token must be unchanged: $\mathbf{x}_{t-1} = \mathbf{x}_t$.
- ▶ Observing an unmasked token at time t fixes the entire history: $\mathbf{x}_{t-1} = \mathbf{x}_t = \dots = \mathbf{x}_0$.

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- ▶ Observing an unmasked token at time t fixes the entire history: $\mathbf{x}_{t-1} = \mathbf{x}_t = \dots = \mathbf{x}_0$.
- ▶ If $\mathbf{x}_t = \mathbf{e}_m$, the previous token may be either clean or masked.
- ▶ With probability ρ_t , masking occurred exactly at step t (so $\mathbf{x}_{t-1} = \mathbf{x}_0$).
- ▶ With probability $(1 - \rho_t)$, the token was already masked earlier (so $\mathbf{x}_{t-1} = \mathbf{e}_m$).

Absorbing Diffusion

Sequence Distribution

$$q(\mathbf{X}_{t-1}|\mathbf{X}_t, \mathbf{X}_0) = \prod_{i=1}^m q(\mathbf{x}_{t-1}^i|\mathbf{x}_t^i, \mathbf{x}_0^i).$$

Each position i has two possible cases:

$$\mathbf{x}_t^i \neq \mathbf{e}_m \Rightarrow \mathbf{x}_{t-1}^i = \mathbf{x}_t^i, \quad \mathbf{x}_t^i = \mathbf{e}_m \Rightarrow \mathbf{x}_{t-1}^i \in \{\mathbf{x}_0^i, \mathbf{e}_m\}.$$

Absorbing Diffusion

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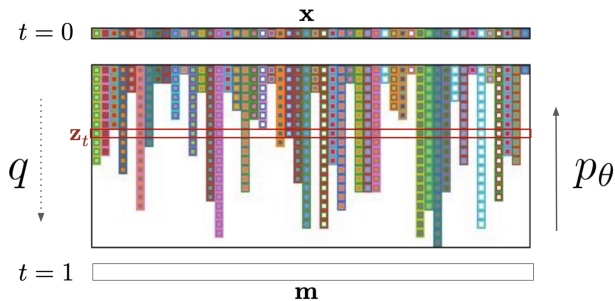
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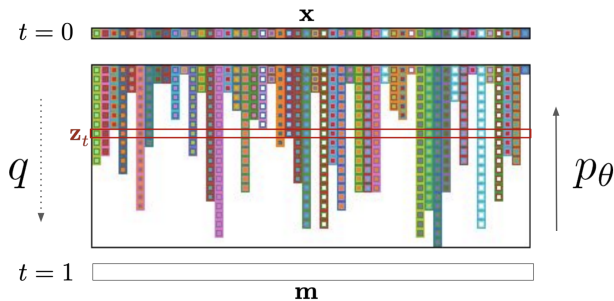
Interpretation

- ▶ The forward process produces **random partial observations** of the clean sequence.
- ▶ If a token is visible at time t , the reverse distribution is deterministic.
- ▶ Unmasked tokens yield a deterministic posterior and therefore contribute only a constant to the ELBO. Therefore, only masked tokens contribute to the training loss.

Absorbing Diffusion

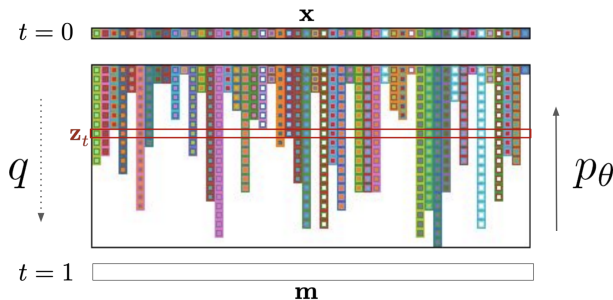


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Absorbing Diffusion



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Objective: sequence-level \mathcal{L}_t

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \sum_{i=1}^m \rho_t[\mathbf{x}_t^i = \mathbf{e}_m] \left[-\log p_\theta(\mathbf{x}_0^i|\mathbf{X}_t) \right] + \text{const}$$

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From Discrete Time to Mask Rate

In absorbing diffusion, the forward process is

$$q(\mathbf{x}_t|\mathbf{x}_0) = \bar{\alpha}_t[\mathbf{x}_t = \mathbf{x}_0] + (1 - \bar{\alpha}_t)[\mathbf{x}_t = \mathbf{e}_m].$$

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$$\lambda_t = 1 - \bar{\alpha}_t \in [0, 1].$$

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- ▶ We can therefore reparameterize the corruption level by

$$t \quad \Rightarrow \quad \lambda \in [0, 1].$$

- ▶ We directly define a family of corrupted distributions indexed by a continuous mask rate λ :

$$q(\mathbf{x}_\lambda|\mathbf{x}_0) = (1 - \lambda)[\mathbf{x}_\lambda = \mathbf{x}_0] + \lambda[\mathbf{x}_\lambda = \mathbf{e}_m].$$

Discrete ELBO Revisited

Recall the per-step ELBO term for absorbing diffusion:

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \sum_{i=1}^m \rho_t[\mathbf{x}_t^i = \mathbf{e}_m] [-\log p_{\theta}(\mathbf{x}_0^i|\mathbf{X}_t)] + \text{const.}$$

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Replacing the discrete index t with the continuous mask rate λ , the training objective becomes

$$\mathcal{L} = \int_0^1 w(\lambda) \mathbb{E}_{q_\lambda(\mathbf{x}_\lambda|\mathbf{x}_0)} \sum_{i=1}^m [\mathbf{x}_\lambda^i = \mathbf{e}_m] [-\log p_\theta(\mathbf{x}_0^i|\mathbf{X}_\lambda)] d\lambda.$$

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Interpretation

Training corresponds to optimizing a **continuous mixture of masked language modeling objectives** with different mask rates.

Algorithm: Masked Diffusion Language Model (MDLM)

Training

1. Sample $\mathbf{X}_0 \sim p_{\text{data}}(\mathbf{X})$ and $\lambda \sim w(\lambda)$.
2. Corrupt the sequence by independent masking:

$$\mathbf{x}_{\lambda}^i = \begin{cases} \mathbf{e}_m, & \text{with prob. } \lambda, \\ \mathbf{x}_0^i, & \text{with prob. } 1 - \lambda, \end{cases} \quad i = 1, \dots, m.$$

3. Predict token distributions in parallel:

$$p_{\theta}(\mathbf{X}_0 | \mathbf{X}_{\lambda}) = \prod_{i=1}^m p_{\theta}(\mathbf{x}_0^i | \mathbf{X}_{\lambda}).$$

4. Compute the masked-CE loss:

$$\mathcal{L}(\theta) = \sum_{i=1}^m [\mathbf{x}_{\lambda}^i = \mathbf{e}_m] [-\log p_{\theta}(\mathbf{x}_0^i | \mathbf{X}_{\lambda})].$$

Algorithm: Masked Diffusion Language Model (MDLM)

Sampling

1. Initialize $\mathbf{X} \leftarrow \mathbf{e}_m \mathbf{1}^\top$ (fully masked).
2. For a decreasing schedule $\lambda_1 > \lambda_2 > \dots > \lambda_L$:
 - 2.1 Predict $p_\theta(\mathbf{x}^i | \mathbf{X})$ for all positions.
 - 2.2 Unmask a subset of positions to reach the next mask rate $\lambda_{\ell+1}$ (e.g., sample tokens for newly-unmasked positions).
3. Return the final sequence \mathbf{X} (fully unmasked).

Outline

1. Discrete Diffusion

From Token to Sequence

Absorbing Diffusion

Continuous-Time Formulation

2. Course Overview

Course Overview: Problem Statement

Goal

Learn a generative model $p_{\theta}(\mathbf{x})$ that matches the data distribution $p_{\text{data}}(\mathbf{x})$.

Three similar lenses

- **Divergence minimization:**

$$\min_{\theta} D(p_{\text{data}} || p_{\theta}) \quad (\text{KL, JS, Wasserstein, etc.})$$

- **Likelihood-based modeling:** maximize $\log p_{\theta}(\mathbf{x})$ (NF, VAE, diffusion-as-VAE).
- **Score-based modeling:** learn $\nabla_{\mathbf{x}} \log p(\mathbf{x})$ (DDPM / NCSN / SDE).

What We Covered: Part 1

Likelihood-based

► Autoregressive (L1):

$$p_{\theta}(\mathbf{x}) = \prod_{i=1}^n p_{\theta}(x_i | \mathbf{x}_{1:i})$$

► Normalizing Flows (L2, L10):

$$\mathbf{x} = \mathbf{f}_{\theta}(\mathbf{z}), \quad \log p_{\theta}(\mathbf{x}) = \log p(\mathbf{z}) + \log \left| \det \frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right|$$

► VAE (L3–L4):

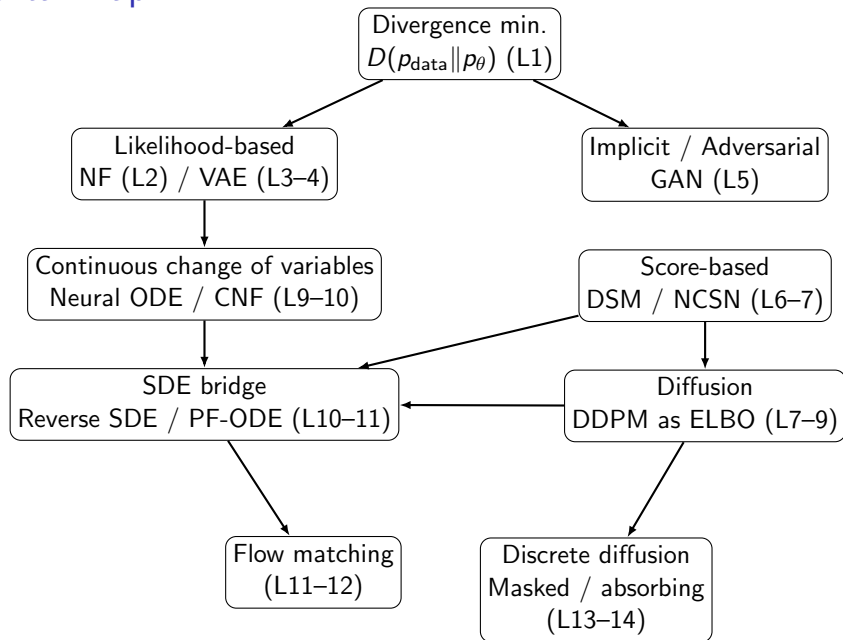
$$\log p_{\theta}(\mathbf{x}) \geq \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}|\mathbf{z})] - \text{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}))$$

What We Covered: Part 2

Implicit / Score-based

- ▶ **GAN (L5)**: implicit p_θ , adversarial learning (close to JSD)
- ▶ **Score matching (L6)**: learn $\mathbf{s}_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$
- ▶ **Diffusion / DDPM (L7–L9)**: forward noising $q(\mathbf{x}_t|\mathbf{x}_{t-1})$ + reverse denoising
- ▶ **SDE / Flow matching (L10–L12)**: reverse SDE \leftrightarrow probability flow ODE, vector field (Neural ODE) / flow matching
- ▶ **Discrete diffusion (L13–L14)**: Markov chain on categorical states

Mental Map



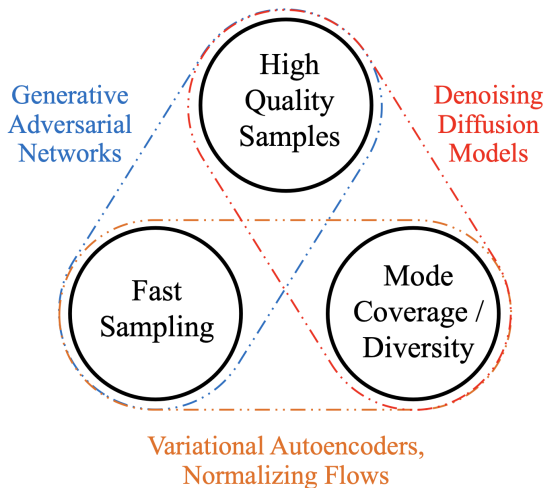
Comparison Cheat-Sheet: Part 1

Family	Likelihood	Training
AR	✓	stable CE
NF	✓	tricky architecture
VAE	lower bound	stable ELBO
GAN	×	unstable/minimax
Diffusion	bound / est.	stable
FM / ODE	est. / bound	stable
Discr. diff.	bound / CE-like	stable

Comparison Cheat-Sheet: Part 2

Family	Sampling	Best for
AR	slow (sequential)	text / discrete
NF	fast (1 step)	exact density, OOD
VAE	fast (1 step)	latent modelling
GAN	fast (1 step)	sharp images
Diffusion	slow (many steps)	high fidelity + diversity
FM / ODE	medium-fast	fewer steps + theory
Discr. diff.	iterative	sequences + bidirectional gen

Generative Learning Trilemma



Xiao Z., Kreis K., Vahdat A. Tackling the generative learning trilemma with denoising diffusion GANs, 2021

Generative Learning Trilemma

Rule of Thumb

- ▶ **Likelihood & Coverage \Rightarrow AR / NF** exact density, no mode dropping, *slow sampling*
- ▶ **Likelihood & Fast Sampling \Rightarrow VAE** tractable bound, fast, *blurry samples*
- ▶ **Sample Quality & Fast Sampling \Rightarrow GAN** sharp samples, *no likelihood, mode collapse*
- ▶ **Quality & Coverage \Rightarrow Diffusion** stable training, high fidelity, *slow sampling*
- ▶ **Quality & Faster Sampling \Rightarrow FM / ODE** fewer steps, continuous flows, *approx. likelihood*
- ▶ **Discrete Structure & Coverage \Rightarrow Discrete Diffusion** stable CE training, parallel denoising, *iterative decoding*

Summary

- ▶ For sequences, the forward process of discrete diffusion factorizes over positions, but reverse process (the model p_θ) conditions on the whole context.
- ▶ In the absorbing case, tokens are either unchanged or masked; so only masked tokens contribute to the ELBO loss.
- ▶ The discrete ELBO reduces to a MLM objective.
- ▶ Reparameterizing time by the mask rate $\lambda \in [0, 1]$ yields a continuous mixture of MLM losses.
- ▶ MDLM sampling performs iterative parallel refinement from fully masked to fully unmasked sequences.
- ▶ No generative model is strictly better than all others: different methods occupy different corners of the generative learning trilemma and come with unavoidable disadvantages.