

AI Applications Lecture 14

Image Generation AI 4: Goals and Scheduling of Diffusion Processes

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Introduction

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Last time, we learned that we can generate low-resolution **latent images** through continuous update steps using **pseudo-random numbers** and a **denoising scheduler**. However, what each update step **aims for** was largely based on intuition. In this lecture, we will explain the **meaning of the scheduler's update equations** and the **design of convergence to the target distribution** by formulating them mathematically and rigorously.

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- Explain how training a **noise estimator** using **data point pairs generated by adding noise** simultaneously solves **two difficulties**: (i) learning from **realistically obtainable data** and (ii) **realizing the target distribution** through a **reverse diffusion process**.
- Explain, through theorems and calculations, in what sense a **denoising scheduler approaches the target distribution with each update**.

Preparation: Mathematical Notations

Notations (1/2) i

- **Definition:** $(\text{LHS}) := (\text{RHS})$: The left-hand side is defined by the right-hand side.

- **Function:** Notation $f : \mathcal{X} \rightarrow \mathcal{Y}$, $y = f(x)$.

- **Vector:**
 - Vectors are column vectors, denoted by bold italic lowercase v .
 - $v = \begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix}^\top \in \mathbb{R}^n$.
 - Standard inner product $\langle u, v \rangle := \sum_{i=1}^n u_i v_i$.
- **Sequence:** $a : [1, n]_{\mathbb{Z}} \rightarrow \mathcal{A}$ is called a sequence of length n .
- **Matrix:** Matrices are bold italic uppercase $A \in \mathbb{R}^{m,n}$. Transpose $A^\top \in \mathbb{R}^{n,m}$.
- **Tensor:** Tensors as multidimensional arrays are written as \underline{A} .

Revisiting the Goal and Steps of the Reverse Diffusion Process

Goal: Conditional Target Distribution

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The **goal** is to achieve **sampling** from a **target distribution** P_c that depends on a text condition $c \in \mathbb{R}^{d_{\text{AllText}}}$. Here,

$$c = (c^{[j]})_{j=1}^n$$

is an output vector sequence from **text encoders**, and although it generally consists of multiple vectors, in this lecture, we treat it as **concatenated into a single vector**.

Invalidity of the Naive Method and Motivation i

The most naive method considered is to **directly output** the **low-resolution latent images that appeared in the training data** corresponding to c , or to add **Gaussian noise** to them.

Invalidity of the Naive Method and Motivation ii

For this reason, we employ the **reverse diffusion process**, which uses the **continuity** and **nonlinearity** of **neural networks** to achieve sampling from a **non-Gaussian** distribution by **push-forward** from a **simple base distribution**.

Review of the Role of Each Step i

In general, the **composition of functions**, such as neural networks, only provides a **point-to-point correspondence between input and output**, not a **distribution** directly.

Discrete-Time Reverse Diffusion and Stability i

We take a discrete time sequence $T = t_0 > t_1 > \cdots > t_K = 0$.

Discrete-Time Reverse Diffusion and Stability ii

For **inference stability**, it is designed such that at each step

$$\|\mathbf{x}_{t_{k+1}} - \mathbf{x}_{t_k}\|_2 \text{ is sufficiently small.} \quad (4)$$

If we write the distribution of \mathbf{x}_{t_k} as P_{t_k} , the ideal is

$$P_{t_0} = \text{StdNormal} \Rightarrow P_{t_1} \Rightarrow \cdots \Rightarrow P_{t_K} \approx P_{\mathbf{c}}. \quad (5)$$

The Non-Triviality of Learning and Forward Noising

What is Observable and What is Missing

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What we can actually obtain is only the **original data** x , which can be regarded as generated from $P_{t_K} = P_c$. The corresponding $x_{t_{K-1}}, \dots, x_{t_0}$ are **not uniquely given**. Therefore, it is necessary to **artificially** construct $x_{t_{K-1}}, \dots, x_{t_0}$. The distributions these follow correspond to $P_{t_{K-1}}, \dots, P_{t_0}$.

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Surveying the situation, we need to satisfy the following **two challenges simultaneously**:

- Making the final distribution P_{t_0} match (or sufficiently approximate) the **target distribution** P_c .
- Being **learnable** through **realistic operations** (possible with available computational resources and data).

Available Probabilistic Tools and Construction of Artificial Distribution Sequence

Constraints on High-Dimensional Distributions i

The only practical distributions that are **directly realizable** in high dimensions and defined by a **small number of parameters** are the **isotropic Gaussian distribution**, the **Cauchy distribution**, and the **uniform distribution within a hypersphere**.

Constructing Random Variables by Linear Combination

Using a sample \mathbf{x} from the original data distribution P_c and an independent $\epsilon \sim \text{StdNormal}_d$, we construct

$$\zeta_{\lambda_{\text{signal}}, \lambda_{\text{noise}}} := \lambda_{\text{signal}} \mathbf{x} + \lambda_{\text{noise}} \epsilon. \quad (6)$$

From a computational cost perspective, if we limit the use to one random vector per data point, the attainable random variables are effectively limited to the form above.

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$$p_{\zeta_{\lambda_{\text{signal}}, \lambda_{\text{noise}}}}. \quad (7)$$

Designing a Smooth Distribution Sequence q_k

To transition **smoothly** from q_0 to q_K , so that the mean and variance move smoothly, we define

$$0 = \bar{\alpha}_0 < \bar{\alpha}_1 < \cdots < \bar{\alpha}_{K-1} < \bar{\alpha}_K = 1 \quad (8)$$

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and set

$$q_k := p_{\zeta_{\sqrt{\bar{\alpha}_k}, \sqrt{1-\bar{\alpha}_k}}}, \quad (9)$$

$$\zeta_k := \sqrt{\bar{\alpha}_k} \mathbf{x} + \sqrt{1-\bar{\alpha}_k} \epsilon, \quad \epsilon \sim \text{StdNormal}_d. \quad (10)$$

Remark

Let the mean and covariance of x be m and V , respectively. Then

$$\mathbb{E}[\zeta_k] = \sqrt{\bar{\alpha}_k} m, \quad (11)$$

$$\text{Cov}(\zeta_k) = \bar{\alpha}_k V + (1 - \bar{\alpha}_k)I. \quad (12)$$

Thus, as k increases, the mean **monotonically** approaches m from 0, and the covariance **monotonically** approaches V from I .

Global Schedule and Training Data Sequence i

The increasing sequence $\{\bar{\alpha}_k\}_{k=0}^K$ used during inference may not be known during training.

Thus, a **sequence of points** $(\zeta^{(i)}, t^{(i)}, \mathbf{x}^{(i)})_{i=1}^m$ is obtained.

Noise Estimator Learning Objective and x Reconstruction i

Using a neural network

$$\hat{\epsilon}_{\theta} : \mathbb{R}^{d_{\text{Latent}}} \times \mathbb{R}^{d_{\text{AllText}}} \times [0, T] \rightarrow \mathbb{R}^{d_{\text{Latent}}} \quad (17)$$

we minimize the following objective function:

$$\min_{\theta} \sum_{i=1}^m \left\| \epsilon^{(i)} - \hat{\epsilon}_{\theta} \left(\zeta^{(i)}, c^{(i)}, t^{(i)} \right) \right\|_2^2. \quad (18)$$

Here, in implementation, $\hat{\epsilon}$ is estimating the **noise**, but due to the **linear relationship**

$$x = \frac{1}{\sqrt{a_t}} \zeta - \frac{\sqrt{1 - \bar{a}_t}}{\sqrt{a_t}} \epsilon, \quad (19)$$

if $\hat{\epsilon}$ is obtained, an estimate of x is also **immediately** obtained.

Goal and Tools: Connection to Scheduler Design

Scheduler Design Goal i

The **goal** is to construct an appropriate function (update equation) and provide a **scheduler** such that its **push-forward distribution**

$$q_0, q_1, \dots, q_{K-1}, q_K$$

gradually approaches the target distribution q_K (i.e., the ideal distribution matching P_c) at each step.

The main tool available is the **noise estimator** $\hat{\epsilon}_\theta$, and the objective function to obtain it is the squared loss above.

Overall Strategy for Denoising Scheduler Construction

Two Main Strategies i

Finally, we construct the **denoising scheduler**. The **goal** is to use the trained noise estimator $\hat{\epsilon}_\theta$ to construct a random variable sequence

$$z_0, z_1, z_2, \dots, z_{K-1}, z_K$$

such that the distribution of each z_k satisfies $\text{Law}(z_k) \approx q_k$.

Two Main Strategies ii

- **Markovian generative transitions:** Choose a joint density $\tilde{q}_{0:K}$ with marginals $\tilde{q}_k = q_k$ and easy conditionals $\tilde{q}_{k+1|k}$. Introduce $\mathbf{u}_k \sim \text{StdNormal}_d$ and set

$$\mathbf{z}_{k+1} = \mathcal{G}_k(\mathbf{z}_k, \hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}, \mathbf{c}, t_k, h_k, \mathbf{u}_k)$$

so that $\text{Law}(\mathbf{z}_{k+1} \mid \mathbf{z}_k)$ matches $\tilde{q}_{k+1|k}$.

Deterministic Scheduling

Revisiting the Goal (Deterministic)

Use $\hat{\epsilon}_\theta$ to construct a deterministic recurrence

$$z_{k+1} = \mathcal{F}_k(z_0, \dots, z_k; \hat{\epsilon}_\theta, \mathbf{c}, t_k, h_k)$$

whose push-forward distribution approaches q_{k+1} . Here h_k is the discrete width in the log-SNR grid.

Log-SNR and Discrete Width

We define the **log-SNR** and width

$$\lambda_k := \log \left(\frac{\sqrt{\bar{\alpha}_k}}{\sqrt{1 - \bar{\alpha}_k}} \right), \quad h_k := \lambda_{k+1} - \lambda_k.$$

Definition: One-Step Method

Definition (One-Step Method Update $\text{Upd1}_{\hat{\epsilon}, \text{coeff}}$)

Given coefficients $\{a_k, b_k\}_{k=0}^{K-1} \subset \mathbb{R}$,

$$\mathbf{z}_{k+1} := a_k \mathbf{z}_k + b_k \hat{\epsilon}_{\theta}(\mathbf{z}_k, \mathbf{c}, t_k).$$

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Remark

Through training,

$$\nabla_{\mathbf{z}} \log q_k(\mathbf{z}) \approx -\frac{1}{\sqrt{1 - \bar{\alpha}_k}} \hat{\epsilon}_{\theta}(\mathbf{z}, \mathbf{c}, t_k)$$

(see cited score-based references).

First-Order KL Expansion for One-Step i

We rewrite the update as

$$\mathbf{z}_{k+1} = \mathbf{z}_k + h_k \mathbf{v}_{\text{upd1}}(\mathbf{z}_k, \lambda_k), \quad \mathbf{v}_{\text{upd1}}(\mathbf{z}, \lambda_k) := \frac{a_k - 1}{h_k} \mathbf{z} + \frac{b_k}{h_k} \hat{\mathbf{e}}_{\theta}(\mathbf{z}, \mathbf{c}, t_k).$$

The ideal connection q_{λ} satisfies the continuity equation

$$\partial_{\lambda} q_{\lambda}(\mathbf{z}) = -\nabla_{\mathbf{z}} \cdot (q_{\lambda}(\mathbf{z}) \mathbf{v}_{\star}(\mathbf{z}, \lambda)).$$

First-Order KL Expansion for One-Step ii

Definition (Updated Distribution and KL)

Let $p_{k+1}^{(1)}$ be the distribution of z_{k+1} from the one-step method, and consider $D_{\text{KL}}(p_{k+1}^{(1)} \parallel q_{k+1})$.

Proposition (First-Order Expansion)

Under regularity and small h_k ,

$$D_{\text{KL}}(p_{k+1}^{(1)} \parallel q_{k+1}) = \frac{h_k^2}{2} \mathbb{E}_{z \sim q_k} \left[\left\| \mathbf{v}_{\text{upd1}}(z, \lambda_k) - \mathbf{v}_*(z, \lambda_k) \right\|_2^2 \right] + \mathcal{O}(h_k^3).$$

Theorem (Optimal Coefficients)

$$a_k^* = \sqrt{\frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} + \mathcal{O}(h_k^2), \quad b_k^* = -\sqrt{\bar{\alpha}_{k+1}} \frac{\sqrt{1 - \bar{\alpha}_k}}{\sqrt{\bar{\alpha}_k}} + \sqrt{1 - \bar{\alpha}_{k+1}} + \mathcal{O}(h_k^2).$$

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Remark

Substituting yields the DDIM deterministic update

$$\mathbf{z}_{k+1} = \sqrt{\frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} \mathbf{z}_k + \left(-\sqrt{\bar{\alpha}_{k+1}} \frac{\sqrt{1 - \bar{\alpha}_k}}{\sqrt{\bar{\alpha}_k}} + \sqrt{1 - \bar{\alpha}_{k+1}} \right) \hat{\epsilon}_{\theta}(\mathbf{z}_k, \mathbf{c}, t_k).$$

Example: Euler ODE Scheduler

Discretizing the ideal drift with forward Euler in λ gives

$$\mathbf{z}_{k+1} = \mathbf{z}_k + h_k \left(\alpha'_k \mathbf{z}_k - \frac{\beta'_k}{\sqrt{1 - \bar{\alpha}_k}} \hat{\epsilon}_{\boldsymbol{\theta}}(\mathbf{z}_k, \mathbf{c}, t_k) \right).$$

This matches the one-step coefficients and principal minimization condition.

Definition (Two-Step Method $\text{Upd2}_{\hat{\epsilon}, \text{coeff}}$)

Given coefficients $\{a_k, b_k^{(0)}, b_k^{(1)}\}$,

$$z_{k+1} = a_k z_k + b_k^{(0)} \hat{\epsilon}_{\theta}(z_k, \mathbf{c}, t_k) + b_k^{(1)} \left(\hat{\epsilon}_{\theta}(z_k, \mathbf{c}, t_k) - \hat{\epsilon}_{\theta}(z_{k-1}, \mathbf{c}, t_{k-1}) \right).$$

Two-Step Method

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Proposition (Second-Order Accuracy)

$$\text{D}_{\text{KL}}\left(p_{k+1}^{(2)} \parallel q_{k+1}\right) = \frac{h_k^3}{2} \mathbb{E}_{q_k} \left[\|\mathbf{a}_2(\mathbf{z})\|_2^2 \right] + \mathcal{O}(h_k^4).$$

Optimal Two-Step Coefficients (DPM++ 2M)

Theorem (Optimal Coefficients)

$$a_k^\star = \sqrt{\frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} + \mathcal{O}(h_k^3), \quad b_k^{(0)\star} = -\frac{\sqrt{\bar{\alpha}_{k+1}}}{\sqrt{\bar{\alpha}_k}} \phi_1(h_k) + \sqrt{1 - \bar{\alpha}_{k+1}}, \quad b_k^{(1)\star} = -\frac{\sqrt{\bar{\alpha}_{k+1}}}{\sqrt{\bar{\alpha}_k}} \phi_2(h_k)$$

with $\phi_1(h) = \frac{e^h - 1}{h}$, $\phi_2(h) = \frac{e^h - 1 - h}{h^2}$.

Stage 1:

$$\tilde{z}_{k+1} = \sqrt{\frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} z_k - \frac{\sqrt{\bar{\alpha}_{k+1}}}{\sqrt{\bar{\alpha}_k}} \phi_1(h_k) \hat{\epsilon}_{\theta}(z_k, \mathbf{c}, t_k) + \sqrt{1 - \bar{\alpha}_{k+1}} \hat{\epsilon}_{\theta}(z_k, \mathbf{c}, t_k).$$

Markovian Scheduling

Goal (Markovian) i

Choose a joint density $\tilde{q}_{0:K}$ with $\tilde{q}_k = q_k$ and tractable $\tilde{q}_{k+1|k}$, and design

$$z_{k+1} = \mathcal{G}_k(z_k, \hat{\epsilon}_\theta, \mathbf{c}, t_k, h_k, \mathbf{u}_k), \quad \mathbf{u}_k \sim \text{StdNormal}_d,$$

such that $\text{Law}(z_{k+1} \mid z_k)$ matches $\tilde{q}_{k+1|k}$.

Local Linear Noising and Gaussian Approximation

Proposition (Gaussian Approximation of Reverse Conditional)

Define

$$\boldsymbol{\xi}_k = \lambda_{\text{signal}} \boldsymbol{\xi}_{k+1} + \delta \boldsymbol{\epsilon}_k, \quad \boldsymbol{\epsilon}_k \sim \text{StdNormal}_d.$$

For sufficiently small $\delta > 0$,

$$p(\boldsymbol{\xi}_{k+1} \mid \boldsymbol{\xi}_k) = \mathcal{N}(\boldsymbol{M}\boldsymbol{\xi}_k, \boldsymbol{\Sigma}) + \mathcal{O}(\delta^2).$$

Definition (Joint of Forward Discrete Diffusion)

In d dimensions, let

$$\boldsymbol{\xi}_K \sim q_K, \quad \boldsymbol{\epsilon}_k \sim \text{StdNormal}_d, \quad \alpha_k := \frac{\bar{\alpha}_{k-1}}{\bar{\alpha}_k},$$

$$\boldsymbol{\xi}_{k-1} = \sqrt{\alpha_k} \boldsymbol{\xi}_k + \sqrt{1 - \alpha_k} \boldsymbol{\epsilon}_k, \quad (k = 1, \dots, K),$$

defining $\tilde{q}_{0:K}$.

Marginals Match the Artificial Path

Theorem (Identity of Marginals)

Under the forward construction, for all k , $\tilde{q}_k = q_k$.

Markovian Update: Definition and Conditional KL

Definition (Markovian Update $\text{MUpd}_{\hat{\epsilon}, \text{coeff}}$)

Given coefficients $\{A_k, B_k, C_k\} \subset \mathbb{R}$,

$$z_{k+1} := A_k z_k + B_k \hat{\epsilon}_{\theta}(z_k, \mathbf{c}, t_k) + C_k \mathbf{u}_k, \quad \mathbf{u}_k \sim \text{StdNormal}_d.$$

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Proposition (First-Order Conditional KL)

Let $\tilde{q}_{k+1|k} = \mathcal{N}(\mu_*(\mathbf{z}), \sigma_*^2 \mathbf{I})$. Then

$$\mathbb{E}_{q_k} \left[D_{\text{KL}}(p_{k+1|k}^{\text{cond}}(\cdot | \mathbf{z}) \parallel \tilde{q}_{k+1|k}(\cdot | \mathbf{z})) \right] = \frac{1}{2} \mathbb{E}_{q_k} \left[\frac{\|\mu_{\text{mupd}} - \mu_*\|_2^2}{\sigma_*^2} + \frac{(\sigma_{\text{mupd}} - \sigma_*)^2}{\sigma_*^2} \right] + \mathcal{O}(h_k^2).$$

Theorem (Optimal Coefficients)

$$A_k^\star = \sqrt{\frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} + \mathcal{O}(h_k^2), \quad B_k^\star = -\sqrt{\bar{\alpha}_{k+1}} \frac{\sqrt{1-\bar{\alpha}_k}}{\sqrt{\bar{\alpha}_k}} + \mathcal{O}(h_k^2), \quad C_k^\star = \sqrt{1 - \frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} + \mathcal{O}(h_k^2).$$

Optimal Markovian Coefficients (DDPM/Euler a)

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Example (DDPM / Euler a)

$$z_{k+1} = \sqrt{\frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} z_k - \sqrt{\bar{\alpha}_{k+1}} \frac{\sqrt{1-\bar{\alpha}_k}}{\sqrt{\bar{\alpha}_k}} \hat{\epsilon}_\theta(z_k, c, t_k) + \sqrt{1 - \frac{\bar{\alpha}_{k+1}}{\bar{\alpha}_k}} u_k.$$

Summary and Next Time

Summary (tied to Learning Outcomes)

- **Data Acquisition for Implicit Distribution Learning:** We constructed an **artificial distribution sequence** q_0, \dots, q_K and corresponding data through forward noising.

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- **Role of Noise Estimator (Reconciliation):** Learning via the objective function achieved the **reconciliation** of two difficult conditions: being learnable from real data and realizing the target distribution via reverse diffusion.

Summary (tied to Learning Outcomes)

- **Data Acquisition for Implicit Distribution Learning:** We constructed an **artificial distribution sequence** q_0, \dots, q_K and corresponding data through forward noising.
- **Role of Noise Estimator (Reconciliation):** Learning via the objective function achieved the **reconciliation** of two difficult conditions: being learnable from real data and realizing the target distribution via reverse diffusion.
- **Proximity of Scheduler:** We showed that by determining the coefficients of deterministic (DDIM/Euler) and stochastic (DDPM/Euler a) updates through moment matching, we **approach** q_{k+1} at each update.

Next Time

Next time, we will discuss **convolutional neural networks** used in image generation AI from an implementation and design perspective (centering on U-Net [1]).

- [1] Olaf Ronneberger, Philipp Fischer, and Thomas Brox.
U-net: Convolutional networks for biomedical image segmentation.
In MICCAI, 2015.