Machine Learning and Optimization

Lecture 23: Diffusion Models I — Learning to Follow the Score

CSCI 4140/6960 — Spring 2026

Course website: `cs.rpi.edu/.../mlandopt.html`

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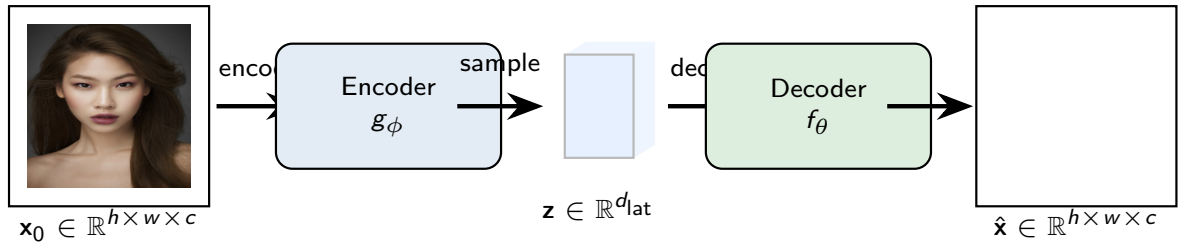
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Motivation for diffusion

What if generation made many small stochastic denoising decisions instead of one large decode decision?

Two Paths to Generation

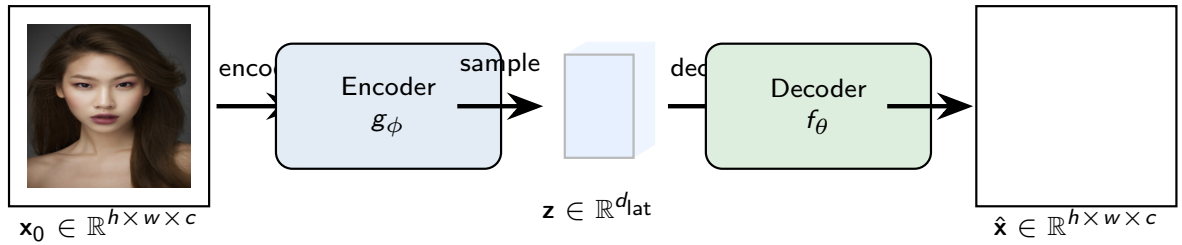
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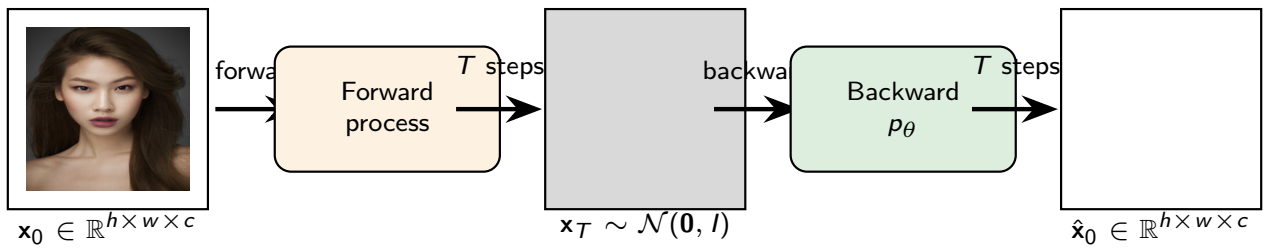
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Diffusion (this lecture): Denoise to generate



Forward process adds noise to reach prior distribution, reverse process removes it to approximately sample from p_{data}.

Forward and Reverse Diffusion Processes

Forward process: Given $\mathbf{x}_0 \sim p_{\text{data}}$, add a little random Gaussian noise to get $\mathbf{x}_1$. Given $\mathbf{x}_{t-1}$ sample $\mathbf{x}_t$ by adding Gaussian noise to get $\mathbf{x}_t$. Do this T times.

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Forward Markov sampling

$\mathbf{x}_t \sim q(\mathbf{x}_t \mid \mathbf{x}_{t-1})$, where $q(\mathbf{x}_t \mid \mathbf{x}_{t-1})$ is the Gaussian density $\mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\,\mathbf{x}_{t-1}, \beta_t I)$

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Backward (learned): Given a sample from the prior $\mathbf{x}_T \sim \mathcal{N}(0, I)$, denoise it using a learned neural network to obtain a sample $\mathbf{x}_{T-1}$. Given sample $\mathbf{x}_t$, denoise it with *the same network* to obtain a sample $\mathbf{x}_{t-1}$. Then $\mathbf{x}_0$ is an approximate sample from p_{data}.

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Backward Markov sampling (learned)

$\mathbf{x}_{t-1} \sim p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) = \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \sigma_\theta^2(\mathbf{x}_t, t))$

Learning Objectives

By the end of this lecture, you should be able to:

1. **Explain** why learning the score of raw data requires knowing $p_{\text{data}}(\mathbf{x})$ (chicken-and-egg problem) and how adding noise makes the score tractable
2. **State** Vincent's theorem: matching conditional scores learns the marginal score because the intractable posterior cancels
3. **Derive** the relationship between noise prediction $\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)$ and the score function
4. **Explain** how the score field connects training (score matching) to sampling (Langevin dynamics)
5. **Recognize** that score matching and likelihood maximization (ELBO) yield the same training objective (full ELBO derivation in appendix)
6. **Implement** Langevin dynamics and DDPM sampling[1]

[1] DDPM = Denoising Diffusion Probabilistic Model (Ho et al., 2020)

Lecture Roadmap

The Sampling Problem: Following the Score

The Forward Process: Multiple Noise Levels

Score Matching: From Objective to Epsilon Prediction

The Training Objective: Two Views

Sampling: Following the Score Field

Implementation and Architecture

Summary

The Sampling Problem: Following the Score

The Score Function

Definition

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$$s(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x})$$

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Question

If we knew $s(\mathbf{x})$, could we generate samples by following it?

A 2D Mixture Example

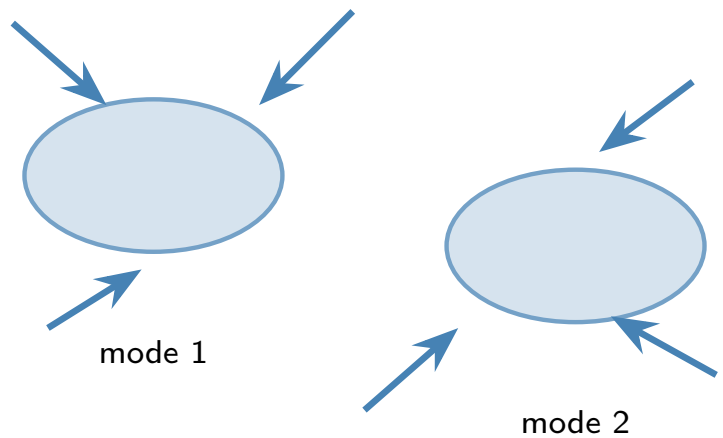
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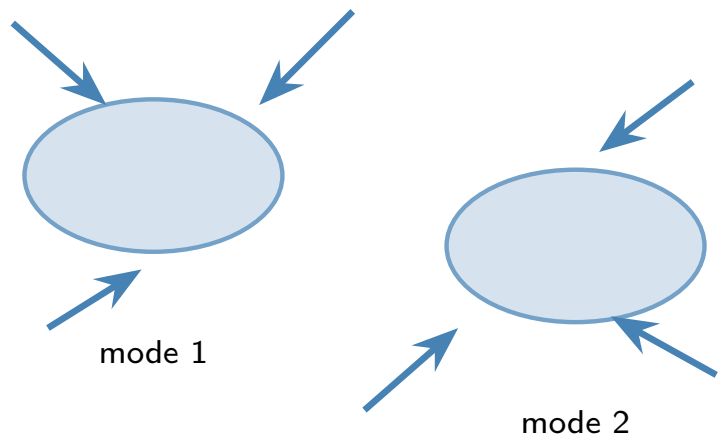
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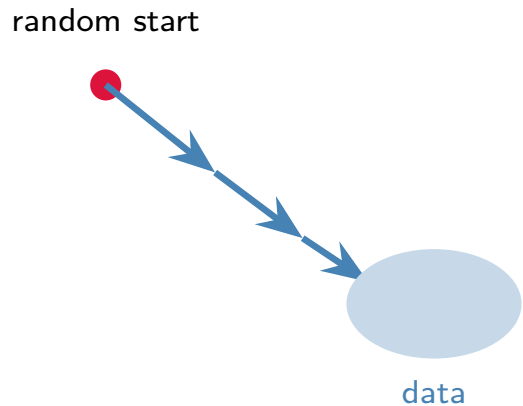
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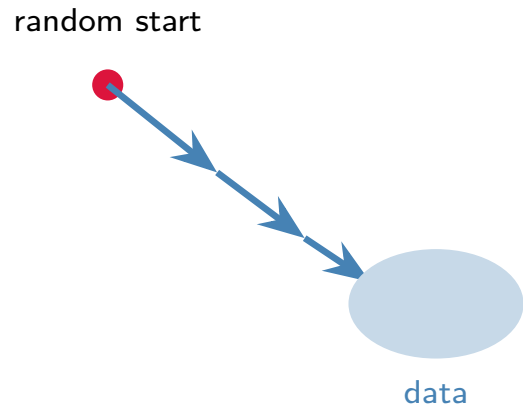
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The problem: We do not know $s(\mathbf{x}) = \nabla \log p_{\text{data}}(\mathbf{x})$ in closed form. We must learn it from data.

Pause and Check: Why the Score?

Question:
Consider a simple 2D Gaussian: $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}; \mathbf{0}, \sigma^2 \mathbf{I})$.

1. What is $\nabla_{\mathbf{x}} p(\mathbf{x})$ (the raw gradient)?
2. What is $\nabla_{\mathbf{x}} \log p(\mathbf{x})$ (the score)?
3. How do they differ in behavior as you move away from the origin?

Think about:

- Which one gives stronger signal far from the mode?
- Which one is more numerically stable?

Why the Score?

For $p(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$:

- $\nabla_{\mathbf{x}} p(\mathbf{x}) = -\frac{\mathbf{x}}{\sigma^2} p(\mathbf{x})$
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Why score, not raw density gradient?

- ∇p vanishes in low-density regions, so guidance disappears far from data
- $\nabla \log p$ preserves directional signal and gives stable long-range drift
- Langevin dynamics uses $\nabla \log p$ and has p as stationary distribution

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Minimize the expected squared error between the learned score and true score:

$$J(\theta) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \left[\| s_\theta(\mathbf{x}) - \nabla \log p_{\text{data}}(\mathbf{x}) \|^2 \right]$$

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We need a way to learn $\nabla \log p_{\text{data}}(\mathbf{x})$ without knowing $p_{\text{data}}(\mathbf{x})$.

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We need a version of p_{data} that is positive *everywhere* in $\mathbb{R}^d$ so the score exists at every point.

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Definition

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Because the Gaussian is positive everywhere, the resulting $p_\sigma(\mathbf{x}) > 0$ for *all* $\mathbf{x} \in \mathbb{R}^d$, and so $\nabla_{\mathbf{x}} \log p_\sigma(\mathbf{x})$ is well-defined everywhere.

Visualizing Smoothing

$\sigma \to 0$



data points

As $\sigma \to 0$, the smoothed distribution approaches the original: $p_\sigma \to p_{\text{data}}$.

So if we can learn $\nabla_{\mathbf{x}} \log p_\sigma(\mathbf{x})$ for a small σ, we get an approximation to the score of the data distribution itself.

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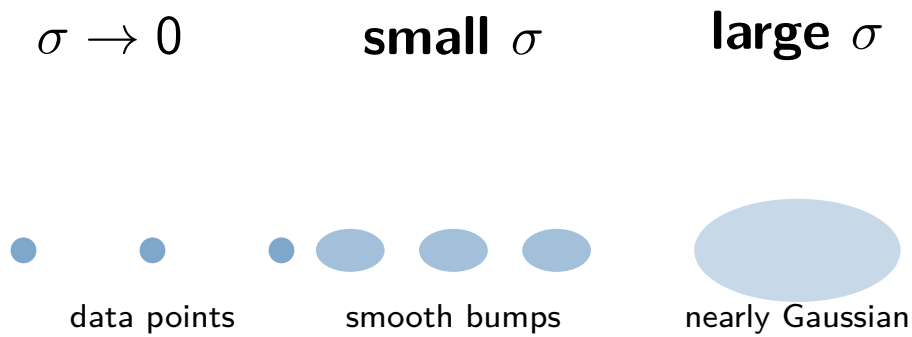
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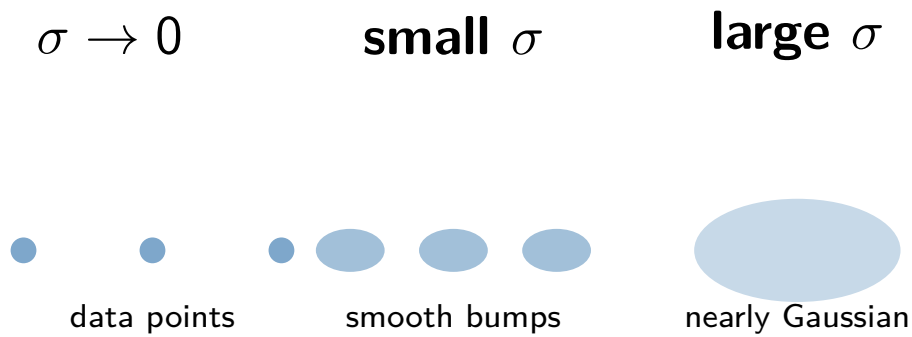
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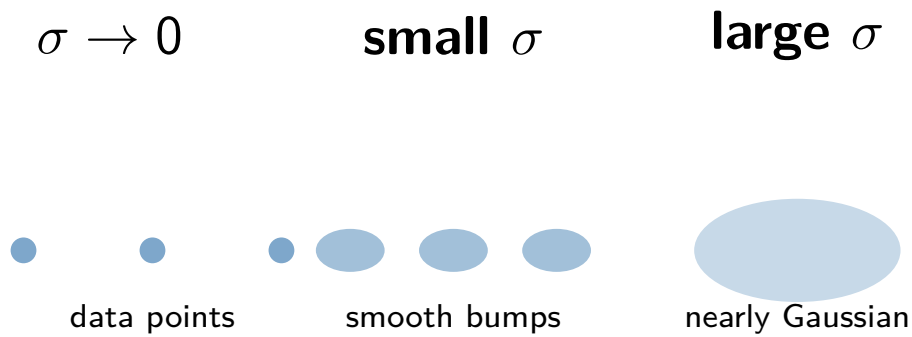


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Over the next several slides we will show that this problem can be solved by a single, elegant mathematical identity: the score of p_{σ} can be expressed in terms of quantities we *can* compute from data.

Setting Up the Derivation

Write $q_\sigma(\mathbf{x} \mid \mathbf{x}_0)$ for the Gaussian noise density centered at $\mathbf{x}_0$:

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We want $\nabla_{\mathbf{x}} \log p_\sigma(\mathbf{x})$. To get there, we will first compute $\nabla_{\mathbf{x}} p_\sigma(\mathbf{x})$ and then use the relationship between the gradient of a function and the gradient of its logarithm.

Computing $\nabla_{\mathbf{x}} p_\sigma(\mathbf{x})$

Differentiating the integral with respect to $\mathbf{x}$:

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(Formally, we also exchange $\nabla_{\mathbf{x}}$ and $\int d\mathbf{x}_0$; this is valid because q_σ is a smooth Gaussian.)

From ∇p to $\nabla \log p$

For any positive function $f(\mathbf{x}) > 0$, the chain rule gives

$$\nabla \log f(\mathbf{x}) = \frac{\nabla f(\mathbf{x})}{f(\mathbf{x})} \qquad \Longleftrightarrow \qquad \nabla f(\mathbf{x}) = f(\mathbf{x})\, \nabla \log f(\mathbf{x})$$

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Now apply the right form to $f = q_\sigma(\cdot \mid \mathbf{x}_0)$ to rewrite $\nabla_{\mathbf{x}} q_\sigma = q_\sigma\, \nabla_{\mathbf{x}} \log q_\sigma$:

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This Is a Conditional Expectation

Look at the formula we just derived:

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The product $p_{\text{data}}(\mathbf{x}_0)\, q_\sigma(\mathbf{x} \mid \mathbf{x}_0)$ is the *joint density* of the pair $(\mathbf{x}_0, \mathbf{x})$: first draw a clean point $\mathbf{x}_0$, then corrupt it to get $\mathbf{x}$.

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Substituting this into our formula:

$$\begin{aligned} \nabla_{\mathbf{x}} \log p_\sigma(\mathbf{x}) &= \int p_\sigma(\mathbf{x}_0 \mid \mathbf{x})\; \nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0)\; d\mathbf{x}_0 \\ &= \mathbb{E}_{p_\sigma(\mathbf{x}_0 \mid \mathbf{x})}\big[\nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0)\big] \end{aligned}$$

What This Formula Says

$$\nabla_{\mathbf{x}} \log p_\sigma(\mathbf{x}) \;=\; \mathbb{E}_{p_\sigma(\mathbf{x}_0|\mathbf{x})}\big[\nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0)\big]$$

In words: the score of the smoothed distribution at a noisy point $\mathbf{x}$ equals the average of the **conditional scores** $\nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0)$, averaged over all the clean points $\mathbf{x}_0$ that could have produced $\mathbf{x}$.

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The remaining question is practical: how do we take this expectation over $\mathbf{x}_0 \mid \mathbf{x}$ during training, when we do not know the posterior $p_\sigma(\mathbf{x}_0 \mid \mathbf{x})$?

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So we train s_θ by minimizing the mean squared error over these joint samples:

$$\mathbb{E}_{\mathbf{x}_0, \boldsymbol{\epsilon}} \left[\left\| s_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0) \right\|^2 \right], \qquad \mathbf{x} = \mathbf{x}_0 + \sigma\boldsymbol{\epsilon}$$

Why This Objective Learns the Right Thing

The function $f(\mathbf{x})$ that minimizes $\mathbb{E}\left[\|Y - f(X)\|^2\right]$ over all measurable f is the conditional expectation $f(\mathbf{x}) = \mathbb{E}[Y \mid X = \mathbf{x}]$.

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Therefore, the network that minimizes this score-matching objective satisfies

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But does this conditional expectation actually equal $\nabla_{\mathbf{x}} \log p_\sigma(\mathbf{x})$, the quantity we want?

Connecting Back: the Conditional Expectation *Is* the Score

On an earlier slide we proved that

$$\nabla_{\mathbf{x}} \log p_\sigma(\mathbf{x}) \;=\; \int p_\sigma(\mathbf{x}_0 \mid \mathbf{x})\, \nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0)\, d\mathbf{x}_0$$

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The right-hand side is, by definition, the conditional expectation of $\nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0)$ given $\mathbf{x}$:

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Training network using the score-matching objective learns the score of the smoothed distribution, without ever computing the posterior $p_\sigma(\mathbf{x}_0 \mid \mathbf{x})$ or the marginal $p_\sigma(\mathbf{x})$!

The Conditional Score in Closed Form

The corruption density is a Gaussian centered at $\mathbf{x}_0$:

$$q_\sigma(\mathbf{x} \mid \mathbf{x}_0) \;=\; \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\!\Big(-\frac{\|\mathbf{x}-\mathbf{x}_0\|^2}{2\sigma^2}\Big)$$

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Now differentiate with respect to $\mathbf{x}$. Recall that $\nabla_{\mathbf{x}}\|\mathbf{x}-\mathbf{x}_0\|^2 = 2(\mathbf{x}-\mathbf{x}_0)$, so:

$$\nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0) \;=\; -\frac{\mathbf{x}-\mathbf{x}_0}{\sigma^2}$$

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We just showed that $\nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x} \mid \mathbf{x}_0) = -(\mathbf{x} - \mathbf{x}_0)/\sigma^2$.

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So predicting the score and predicting the noise are the same problem, up to a factor of $-1/\sigma$.

The Denoising Score Matching Objective

Combining everything: we train a noise-prediction network $\boldsymbol{\epsilon}_\theta(\mathbf{x}, \sigma)$ to minimize

$$\mathbb{E}_{\mathbf{x}_0 \sim p_{\text{data}},\, \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_0 + \sigma \boldsymbol{\epsilon},\ \sigma) \right\|^2 \right]$$

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This is **denoising score matching** (Vincent, 2011): learning the score by learning to denoise.

The Forward Process: Multiple Noise Levels

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So we want a **sequence of noise levels** $\sigma_1 < \sigma_2 < \cdots < \sigma_T$, and a single network $\boldsymbol{\epsilon}_\theta(\mathbf{x}, t)$ trained to predict the noise at every level t.

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At a large noise level, the score field is smooth and easy to follow—it gives us the coarse structure (where are the modes?).

At smaller noise levels, the score field captures finer detail—it sharpens our samples.

So we want a **sequence of noise levels** $\sigma_1 < \sigma_2 < \cdots < \sigma_T$, and a single network $\boldsymbol{\epsilon}_\theta(\mathbf{x}, t)$ trained to predict the noise at every level t.

At sampling time, we start at $t = T$ (heavy noise) and progressively denoise down to $t = 1$ (light noise). This is the core idea of diffusion models.

Defining the Forward Process

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At each step, the transition is:

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There are two things to explain here: why do we *scale down* $\mathbf{x}_{t-1}$ by $\sqrt{1-\beta_t}$, and why is the noise scaled by $\sqrt{\beta_t}$?

Why the Scaling?

If we just added noise without scaling—say $\mathbf{x}_t = \mathbf{x}_{t-1} + \sqrt{\beta_t}\,\boldsymbol{\epsilon}_t$—then the variance of $\mathbf{x}_t$ would grow at every step:

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If $\mathbf{x}_{t-1}$ had unit variance, then $\mathrm{Var}(\mathbf{x}_t) = 1 - \beta_t + \beta_t = 1$. The variance is preserved at each step. Eventually, the signal is fully replaced by noise and $\mathbf{x}_T \approx \mathcal{N}(\mathbf{0}, \mathbf{I})$.

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

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At each step, the mean of $\mathbf{x}_t$ is a slight shrinkage of $\mathbf{x}_{t-1}$, and the variance is β_t (a small number).

Because each step only depends on $\mathbf{x}_{t-1}$ (not on $\mathbf{x}_{t-2}, \ldots, \mathbf{x}_0$), the full forward process $q(\mathbf{x}_{1:T} \mid \mathbf{x}_0)$ is a Markov chain:

$$q(\mathbf{x}_{1:T} \mid \mathbf{x}_0) \;=\; \prod_{t=1}^{T} q(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

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The derivation uses one basic property of Gaussians that we will work through carefully.

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An equivalent restatement: if $\boldsymbol{\epsilon}, \boldsymbol{\epsilon}'$ are independent draws from $\mathcal{N}(\mathbf{0}, \mathbf{I})$, then

$$\sigma_1\,\boldsymbol{\epsilon} + \sigma_2\,\boldsymbol{\epsilon}' \;\sim\; \mathcal{N}\big(\mathbf{0},\; (\sigma_1^2 + \sigma_2^2)\,\mathbf{I}\big) \;=\; \sqrt{\sigma_1^2 + \sigma_2^2}\;\boldsymbol{\epsilon}''$$

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where $\boldsymbol{\epsilon}'' \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ is a single fresh draw.

Two independent Gaussian noise terms can always be replaced by a single Gaussian whose variance is the sum of the two variances.

Deriving the Accumulated Effect: Two Steps

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\end{aligned}$$

Since $\boldsymbol{\epsilon}_1$ and $\boldsymbol{\epsilon}_2$ are independent standard Gaussians, the underbraced term has variance $\alpha_2(1-\alpha_1) + (1-\alpha_2) = 1 - \alpha_1\alpha_2$.

So we can replace it by $\sqrt{1-\alpha_1\alpha_2}\,\boldsymbol{\epsilon}$ for a single $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$:

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This is enormously useful: to generate a training example at any level t, we only need one multiplication, one addition, and one random draw—no chain simulation required.

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For training, this is perfectly fine: we only need the marginal at one randomly chosen t. The joint distribution matters for sampling (the reverse process), which we will address later.

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An alternative is the **cosine schedule** (Nichol & Dhariwal, 2021), which spends more steps at low noise levels where the fine details of the data are being resolved.

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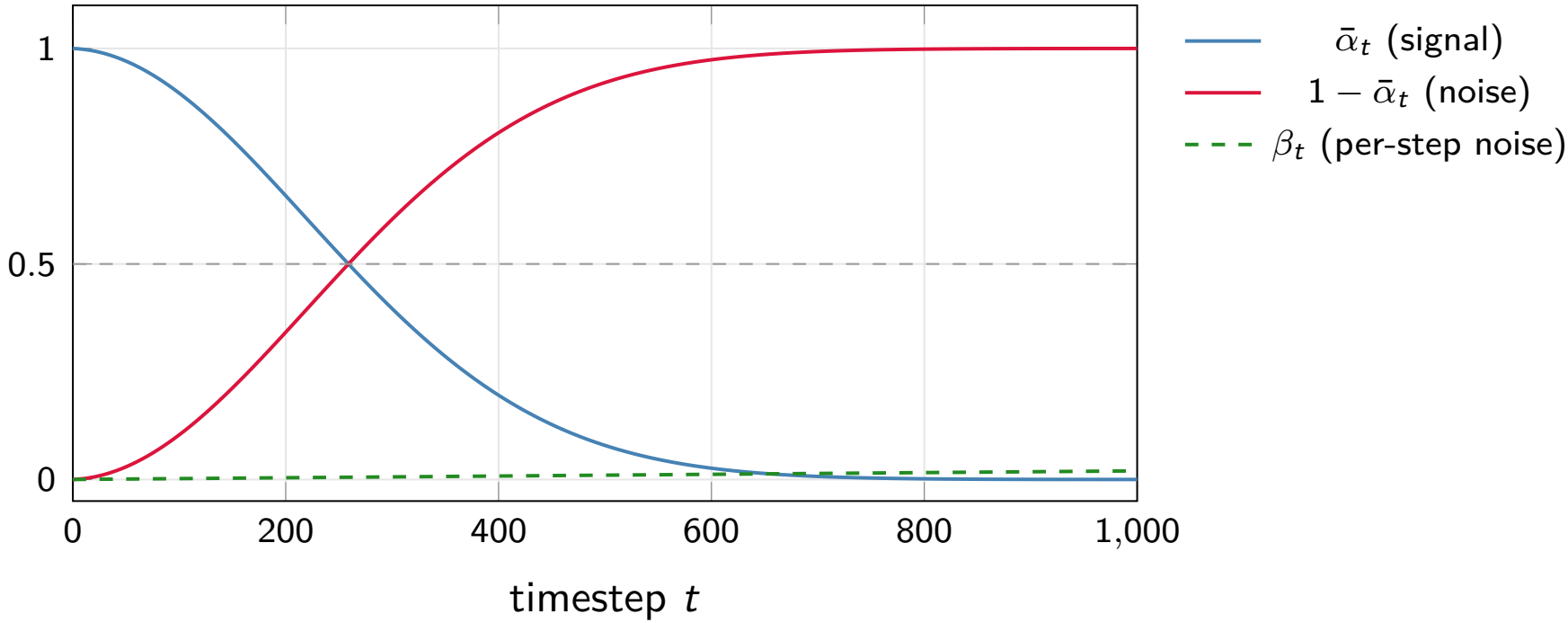
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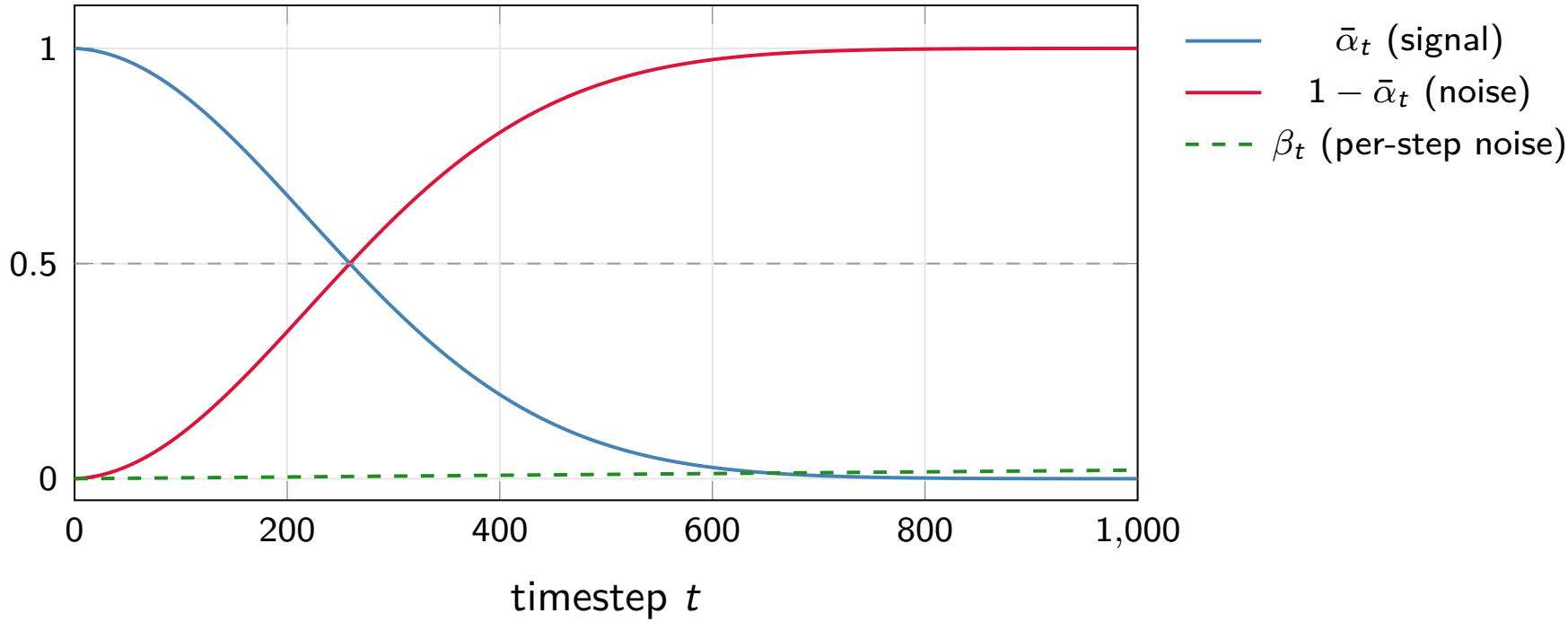
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What matters is not β_t directly, but the *cumulative* quantities $\bar{\alpha}_t$ and $1 - \bar{\alpha}_t$, since those determine how much signal and noise remain at level t.

Visualizing the Schedule



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When $\bar{\alpha}_t \approx 1$, the signal dominates: $\mathbf{x}_t \approx \mathbf{x}_0$, so the noise $\boldsymbol{\epsilon}$ is a small perturbation that is relatively easy to predict. When $\bar{\alpha}_t \approx 0$, the noise dominates: $\mathbf{x}_t \approx \boldsymbol{\epsilon}$, and the score is approximately $-\mathbf{x}_t$, which is trivial. Near the crossover, signal and noise are comparable, so the network must disentangle the two—this is the hardest regime.

Signal-to-Noise Ratio

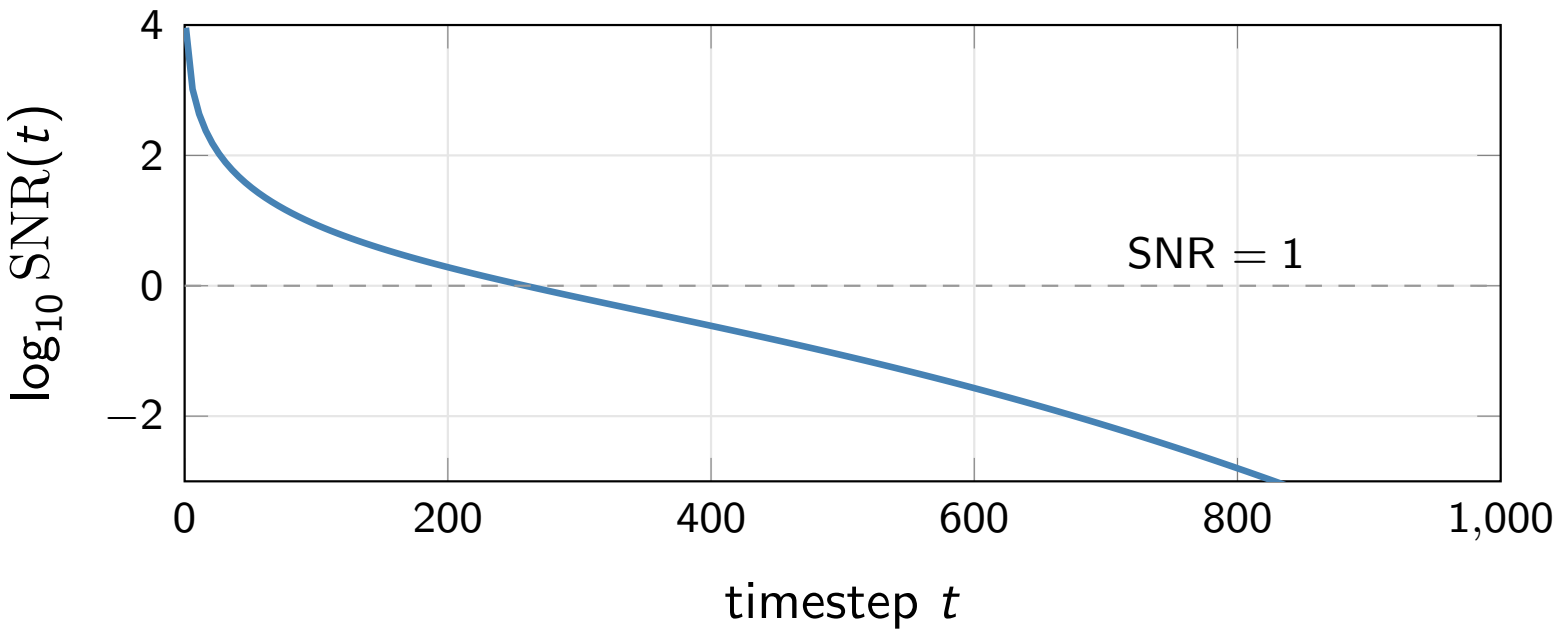
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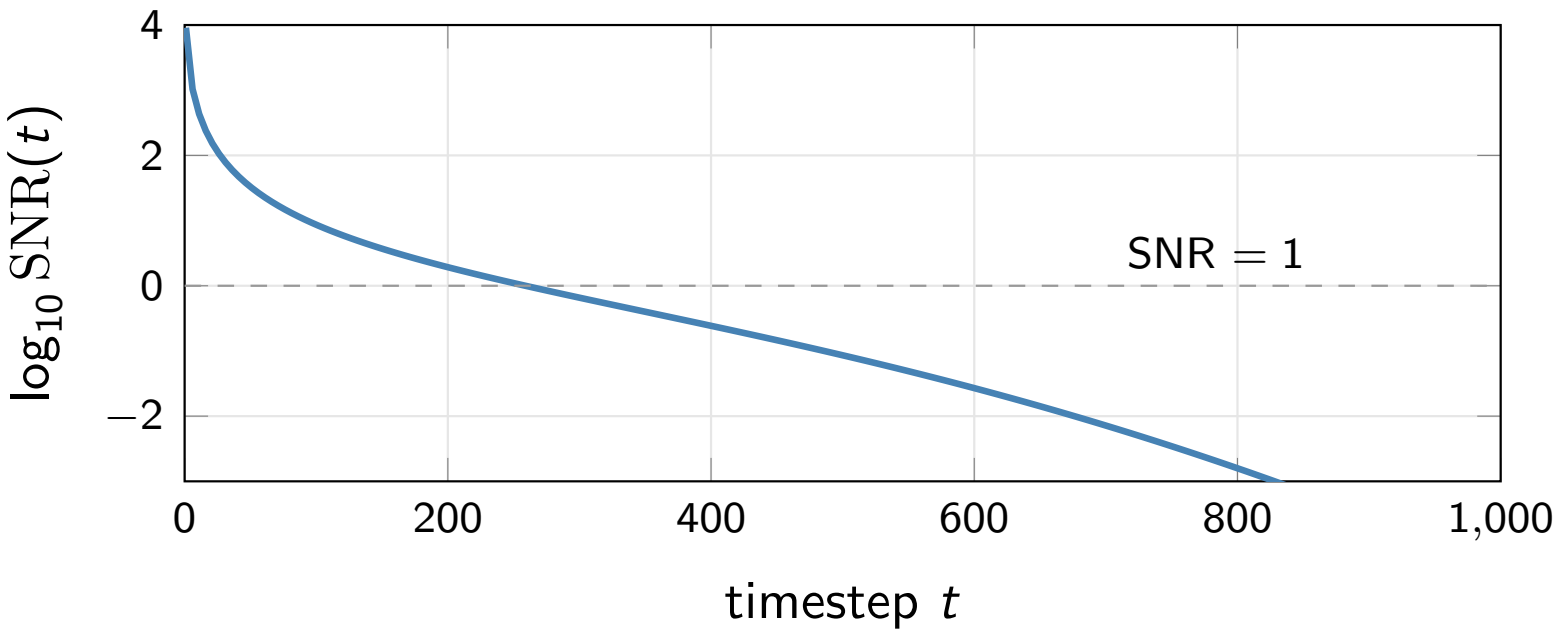
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At early steps, $\mathrm{SNR} \gg 1$: signal dominates. At late steps, $\mathrm{SNR} \ll 1$: noise dominates. The log-SNR drops roughly linearly for the linear schedule.

What the Marginals Look Like

Since $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\,\boldsymbol{\epsilon}$, the marginal $q_t(\mathbf{x}_t)$ is the data distribution convolved with Gaussian noise of variance $1-\bar{\alpha}_t$, and rescaled by $\sqrt{\bar{\alpha}_t}$.

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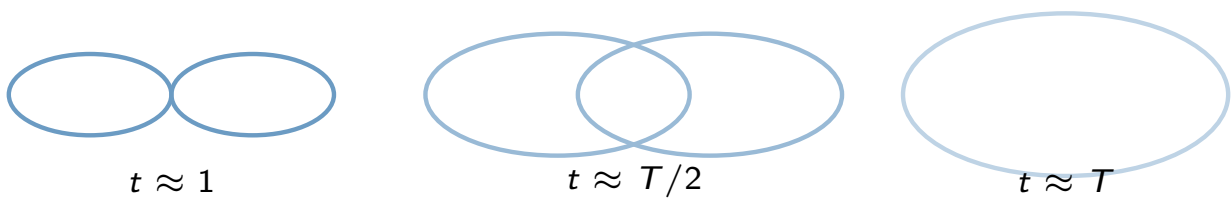
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Single-σ setting	**Forward-process setting**
$\mathbf{x} = \mathbf{x}_0 + \sigma\boldsymbol{\epsilon}$	$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\,\boldsymbol{\epsilon}$
noise variance $= \sigma^2$	noise variance $= 1 - \bar{\alpha}_t$
smoothed density $p_\sigma(\mathbf{x})$	marginal density $q_t(\mathbf{x}_t)$
$\nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x}\|\mathbf{x}_0) = -\boldsymbol{\epsilon}/\sigma$	$\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t\|\mathbf{x}_0) = -\boldsymbol{\epsilon}/\sqrt{1-\bar{\alpha}_t}$

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Every identity we derived—the conditional score formula, the noise-prediction equivalence, the denoising score matching objective—transfers to each noise level t by the substitution $\sigma^2 \leftrightarrow 1 - \bar{\alpha}_t$.

Score Matching: From Objective to Epsilon Prediction

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The conditional score depends only on $\boldsymbol{\epsilon}$.

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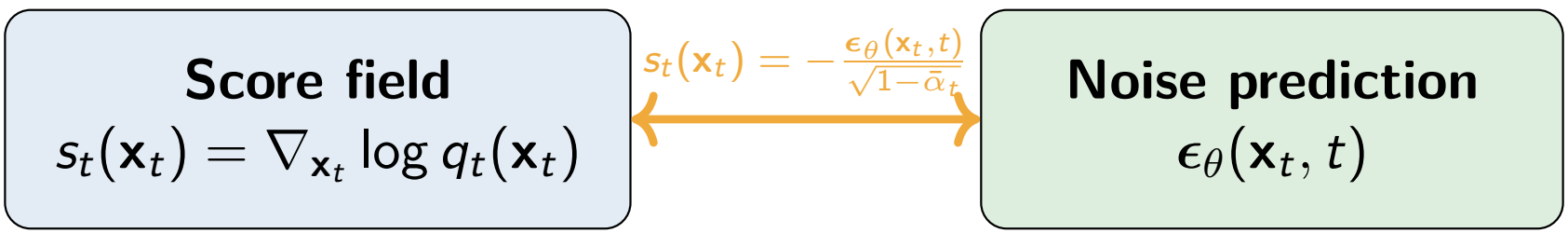
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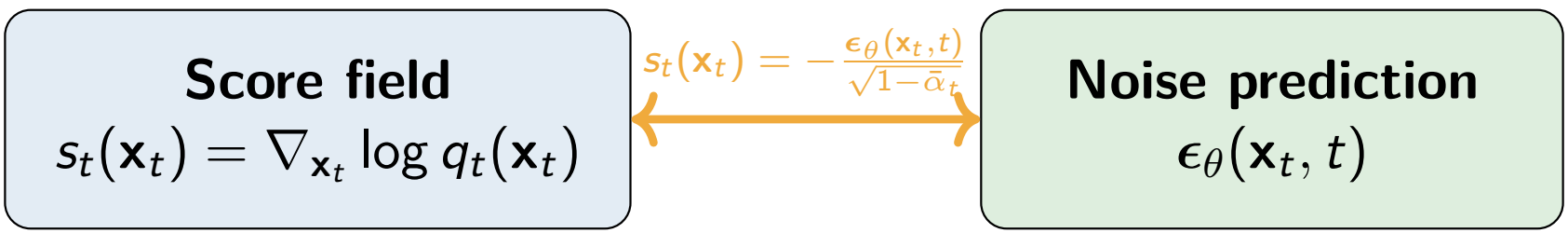
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The Training Objective

Denoising score matching loss:

$$\mathcal{L}_{\text{DSM}} = \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}} \left[\| \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t|\mathbf{x}_0) - s_\theta(\mathbf{x}_t, t) \|^2 \right]$$

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In other words, $\mathcal{L}_{\text{simple}}$ is score matching in disguise: predicting the noise *is* learning the score field, just in a more convenient parameterization. So score-matching can be achieved by denoising.

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Algorithm: DDPM Training (noise-prediction form)

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Repeat:

1. Sample $\mathbf{x}_0 \sim p_{\text{data}}$ (clean training example)
2. Sample $t \sim \text{Uniform}\{1, \ldots, T\}$ (choose noise level)
3. Sample $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ (known target noise)
4. Form $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\,\boldsymbol{\epsilon}$ (forward corruption in one shot)
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The loop itself is short. All the conceptual work—choosing the noise schedule, parameterizing the score via ϵ-prediction, using the one-shot formula for $\mathbf{x}_t$—is already baked into these five lines.

The Training Objective: Two Views

Two Perspectives on the Training Objective

From score matching, we derived the objective

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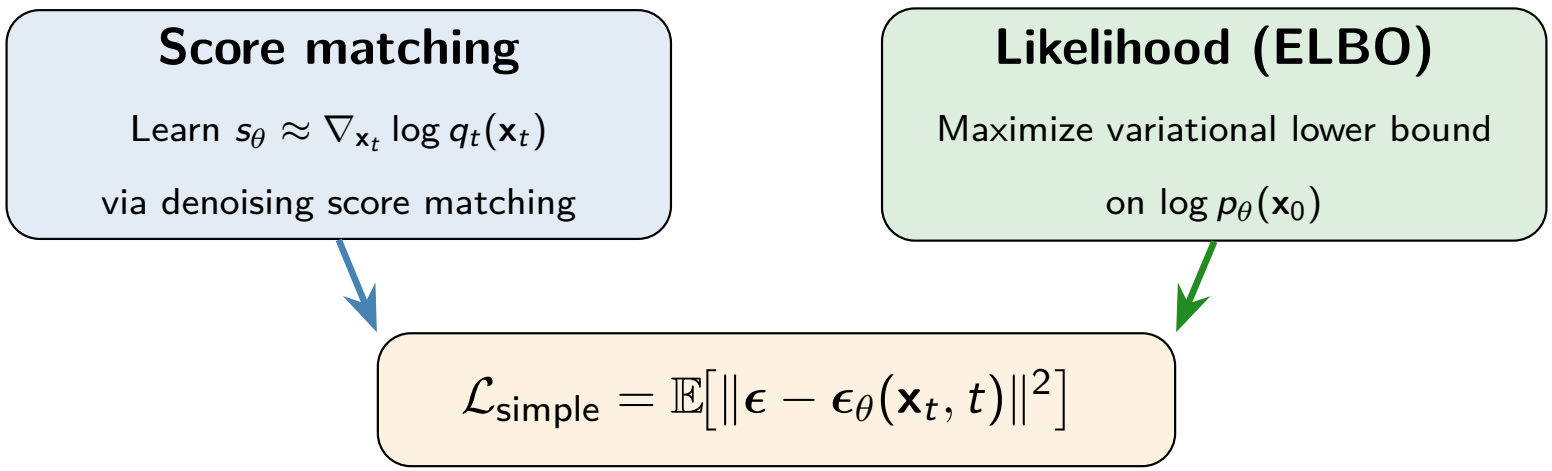
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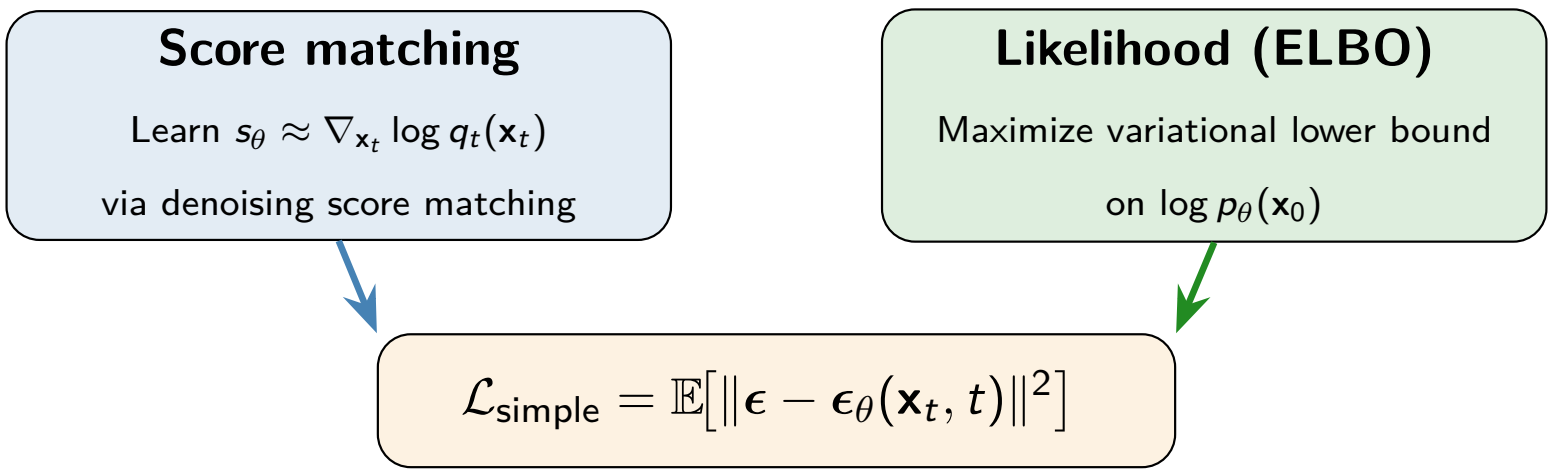


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The full ELBO derivation in given in the appendix. Next: the key ingredients from the likelihood view needed for sampling.

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The mean $\tilde{\mu}_t$ is a weighted average of $\mathbf{x}_0$ and $\mathbf{x}_t$: when noise is low (small t), it trusts $\mathbf{x}_0$ when noise is high (large t), it relies more on $\mathbf{x}_t$.

From Matching to Noise Prediction

We model the reverse process as $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mu_\theta(\mathbf{x}_t, t),\ \tilde{\beta}_t\,\mathbf{I})$, fixing the variance to match the forward posterior and learning only the mean.

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Parameterizing via $\boldsymbol{\epsilon}_\theta$:

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\,\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right).$$

Minimizing $\mathcal{L}_t$ is then (up to a constant factor) the same as minimizing $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\|^2$.

Two Roads, One Objective

Perspective	**Guarantee**	**Design choices**
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ELBO (appendix)	Maximizes likelihood bound	Gaussian p_θ, matched var.

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Both perspectives yield

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t,\,\mathbf{x}_0,\,\boldsymbol{\epsilon}}\left[\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right\|^2\right].$$

Two Roads, One Objective

Perspective	**Guarantee**	**Design choices**
Score matching	Learns $\nabla \log q_t$	ϵ-parameterization
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$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t,\,\mathbf{x}_0,\,\boldsymbol{\epsilon}}\left[\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right\|^2\right].$$

What this means for practice:

- Predicting noise *is* learning the score field
- Learning the score field *is* maximizing a likelihood bound
- The same $\boldsymbol{\epsilon}_\theta$ serves both training and sampling

Sampling: Following the Score Field

Intuition: Score-Guided Sampling

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This is the template DDPM follows: drift toward data + controlled noise.

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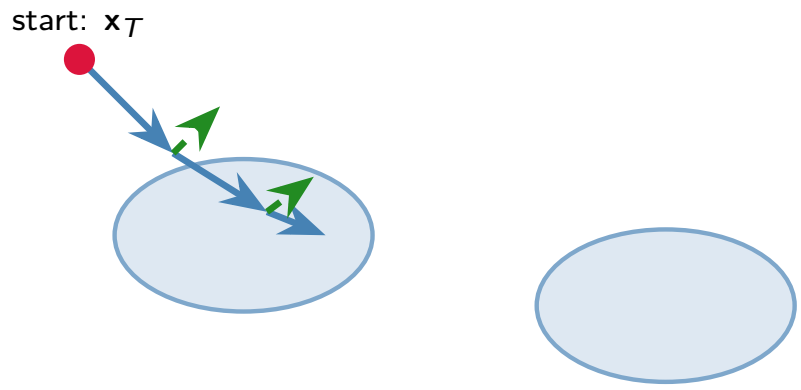
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The difference from pure Langevin: μ_θ is derived by matching the forward posterior mean and the noise level σ_t decreases as we denoise.

What DDPM Does Geometrically

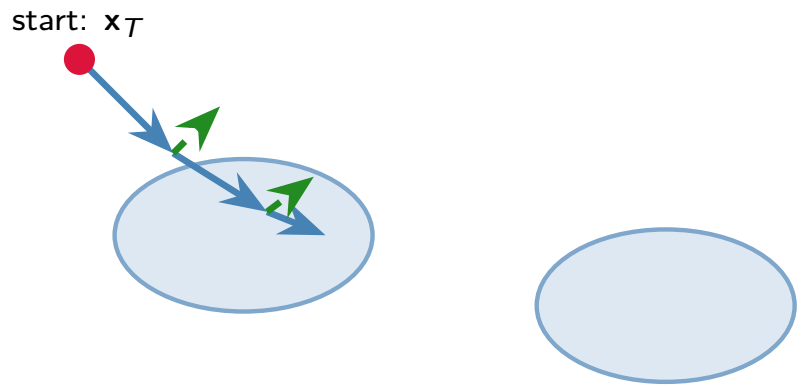
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As t decreases, the noise level σ_t shrinks and the trajectory converges.

The DDPM Sampling Algorithm

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2. For $t = T, T-1, \ldots, 1$:

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What the terms do:

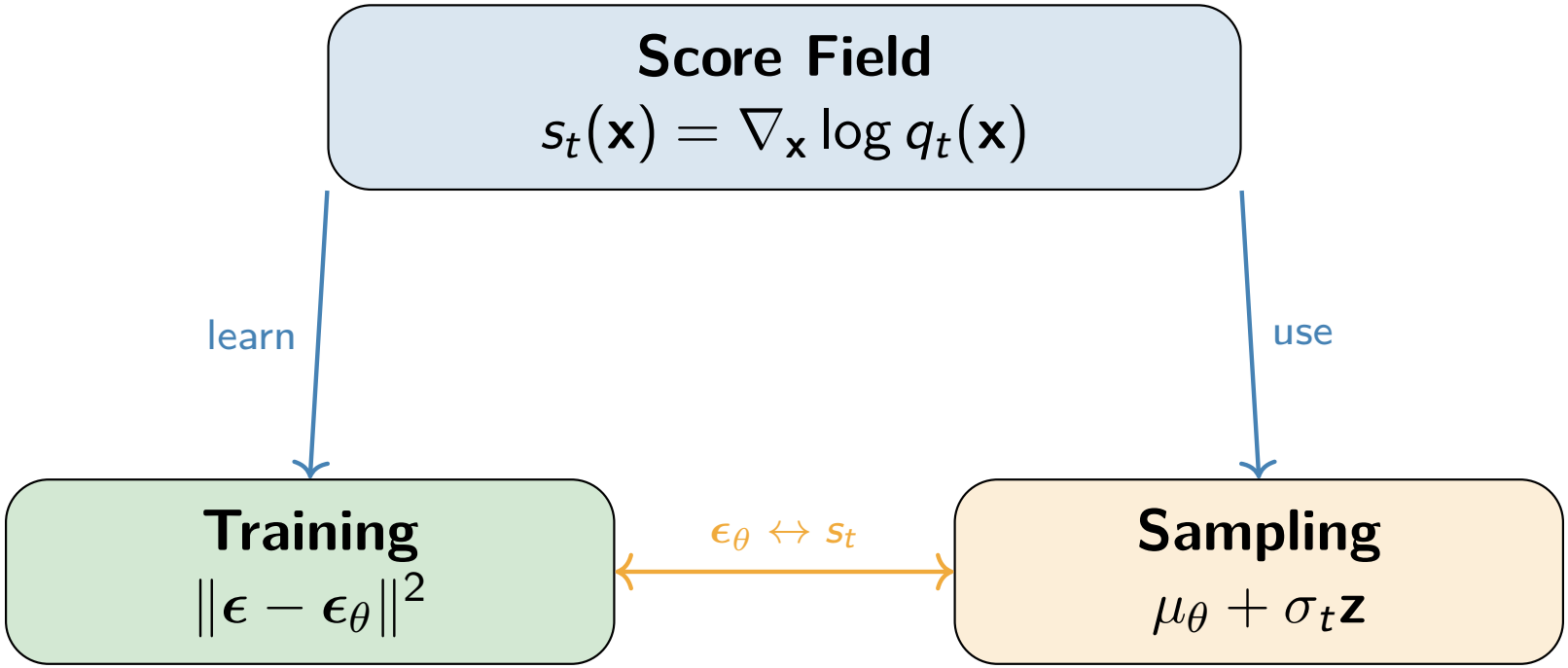
- **Mean μ_θ:** Uses predicted noise ϵ_θ to estimate the cleaner $\mathbf{x}_{t-1}$
- **Variance $\sigma_t^2 = \tilde{\beta}_t$:** Matches the forward posterior variance we computed earlier

The Whole Picture

Everything connects through the score field:

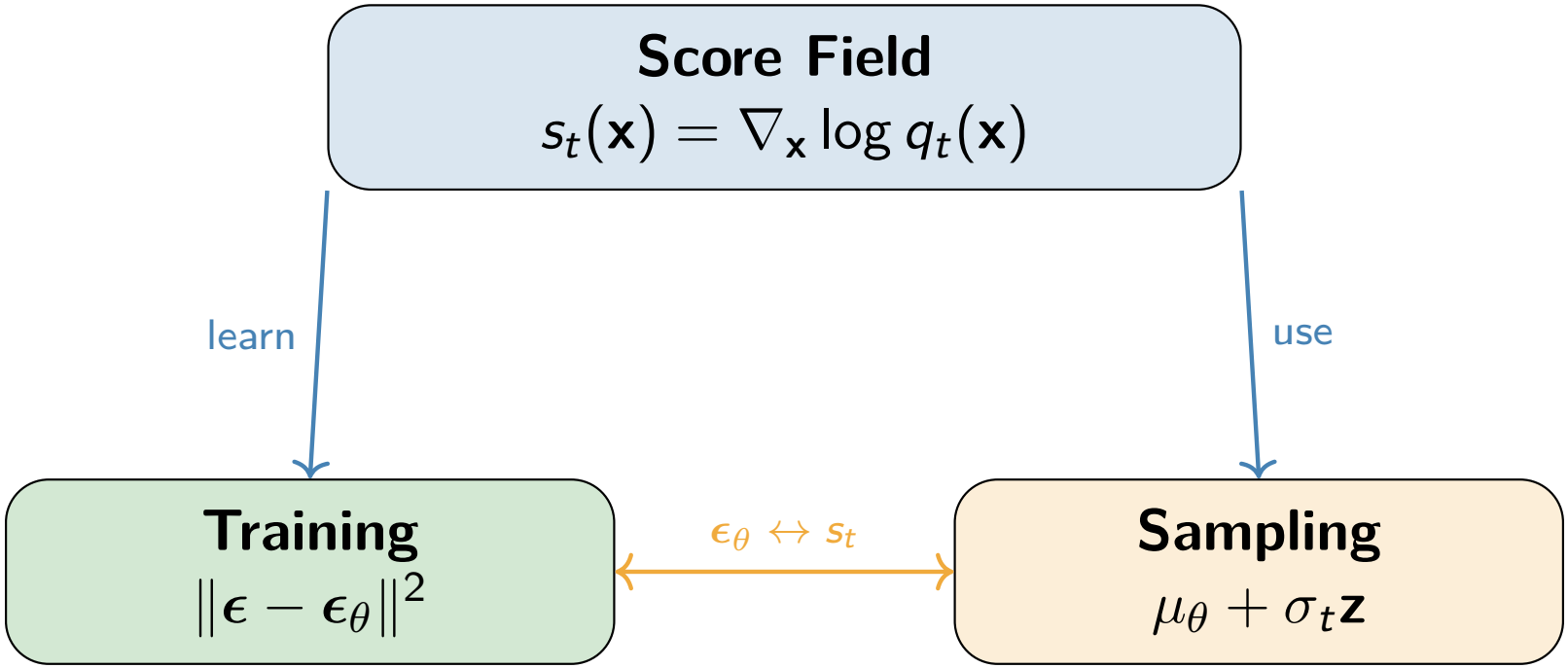
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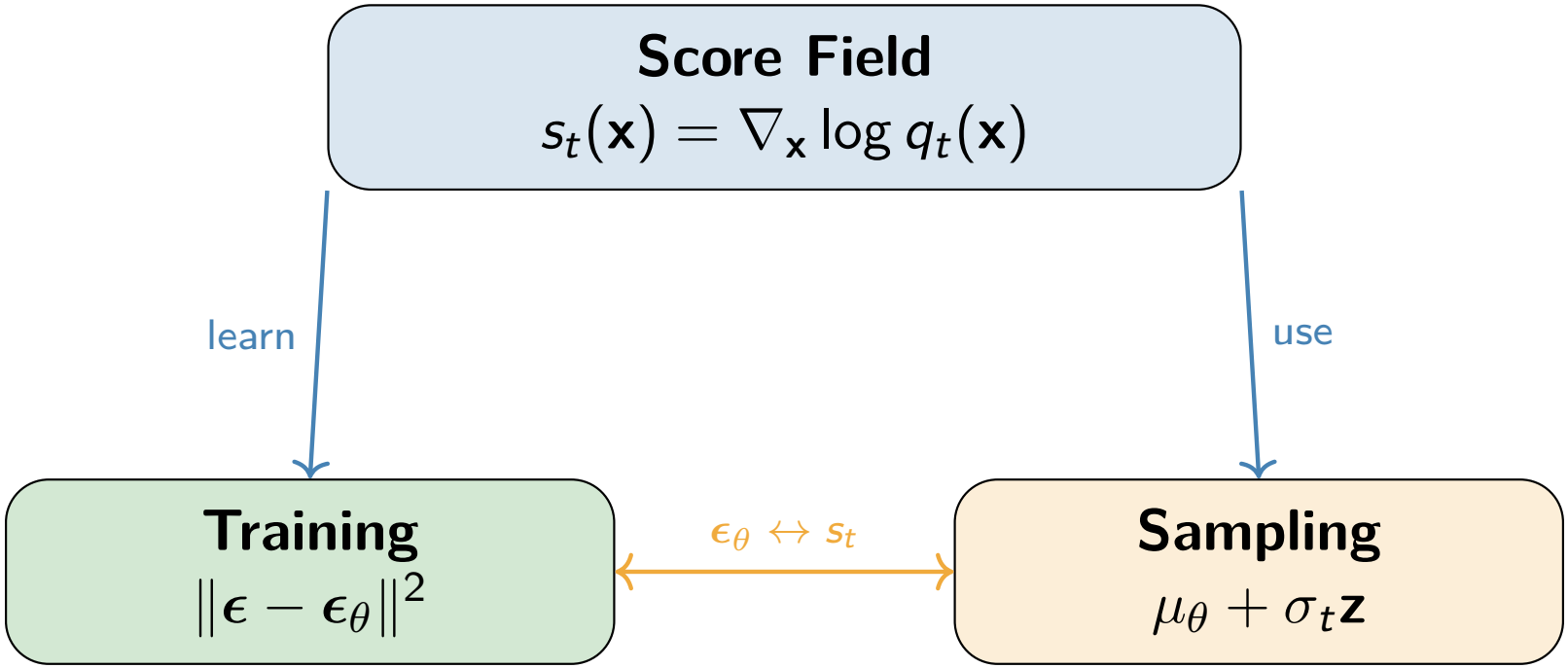


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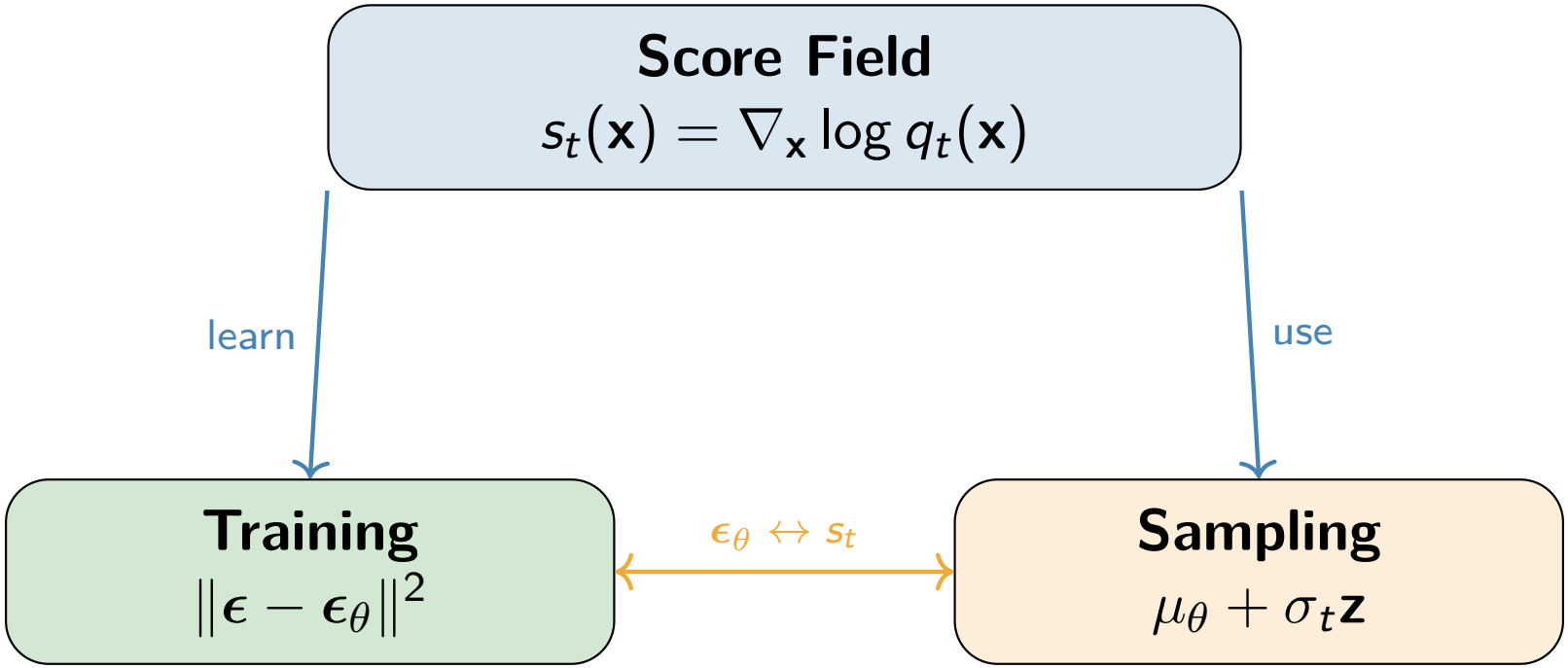


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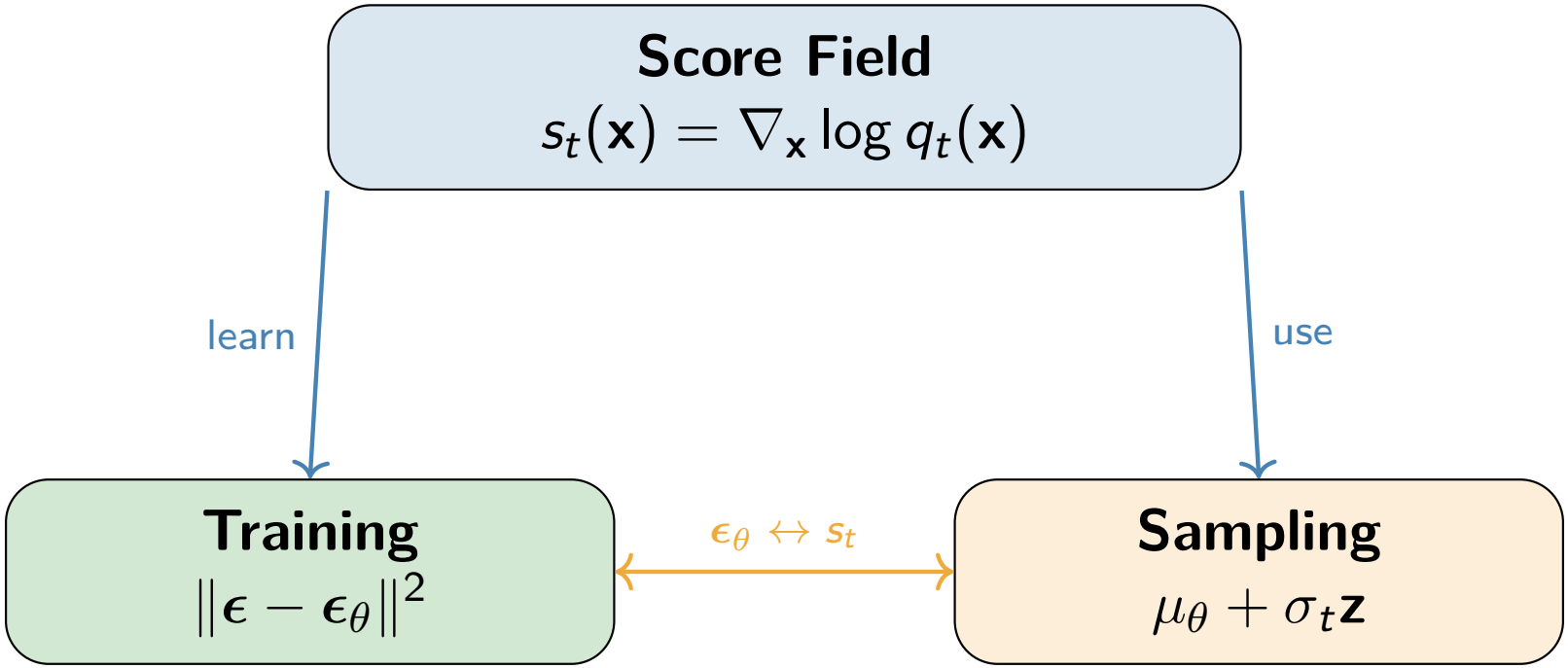


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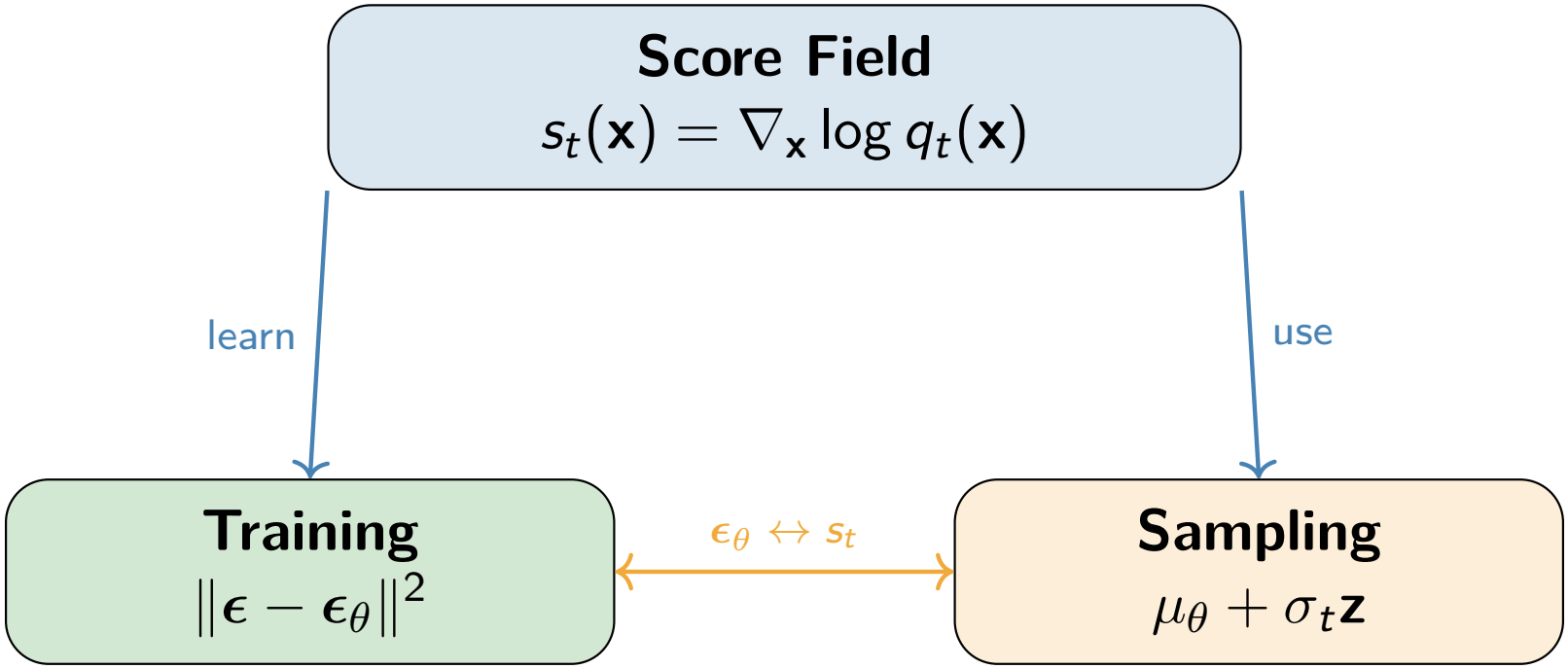


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Implementation and Architecture

Designing the network ϵ_θ

We need to learn $\epsilon_\theta : \mathbb{R}^{h \times w \times c} \times \{1, \ldots, T\} \to \mathbb{R}^{h \times w \times c}$ — taking noisy image $\mathbf{x}_t$ and timestep t, predicting the noise ϵ added to $\mathbf{x}_0$. Two requirements shape the architecture.

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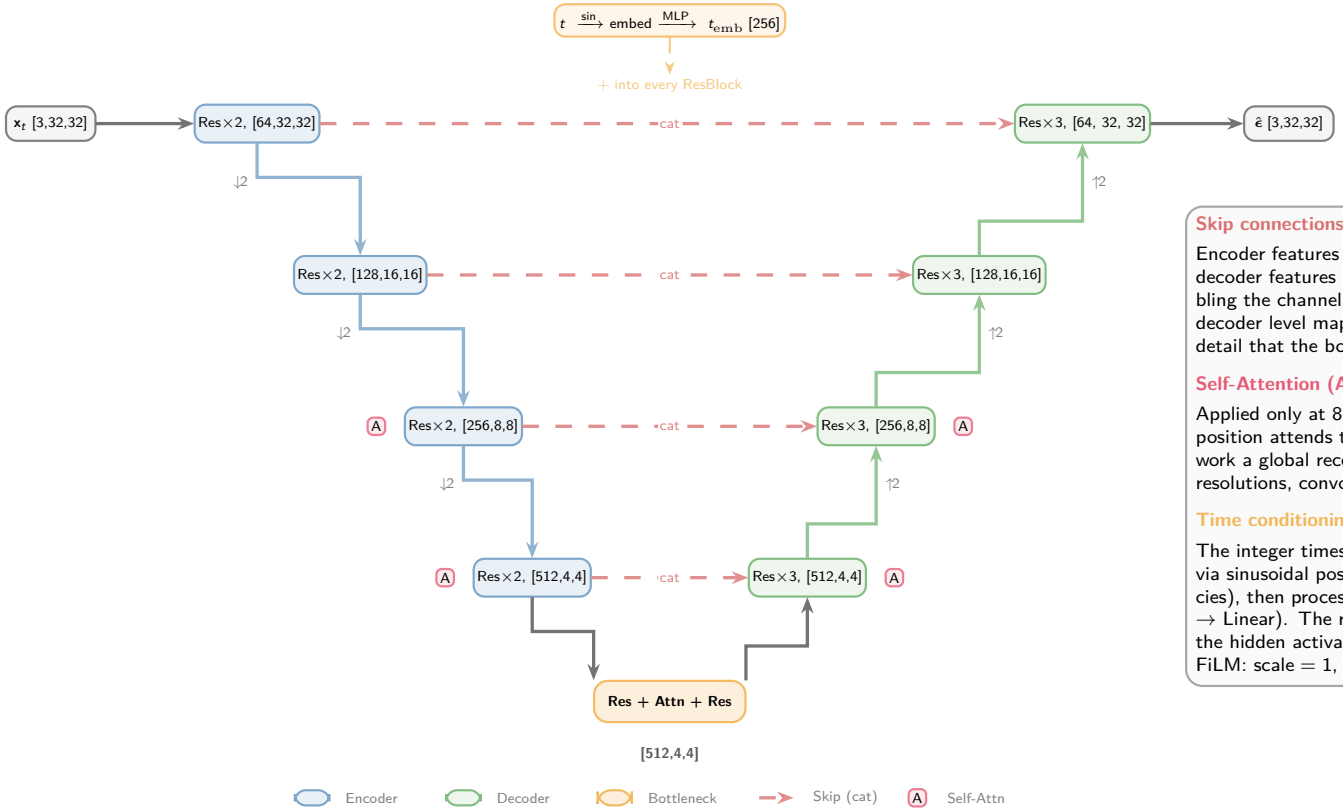
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Behavior must adapt to the noise level t. We need a mechanism to change the network's behavior depending on t.

Our solution is to encode t as a **time embedding** t_{emb} and inject it into every **ResBlock** in the U-Net, changing the features it extracts.

DiffusionUNet Architecture



Skip connections

Encoder features are concatenated (channel axis) with decoder features at the same spatial resolution, doubling the channel count. The first ResBlock of each decoder level maps $2C \to C$. This preserves fine spatial detail that the bottleneck alone would lose.

Self-Attention (A)

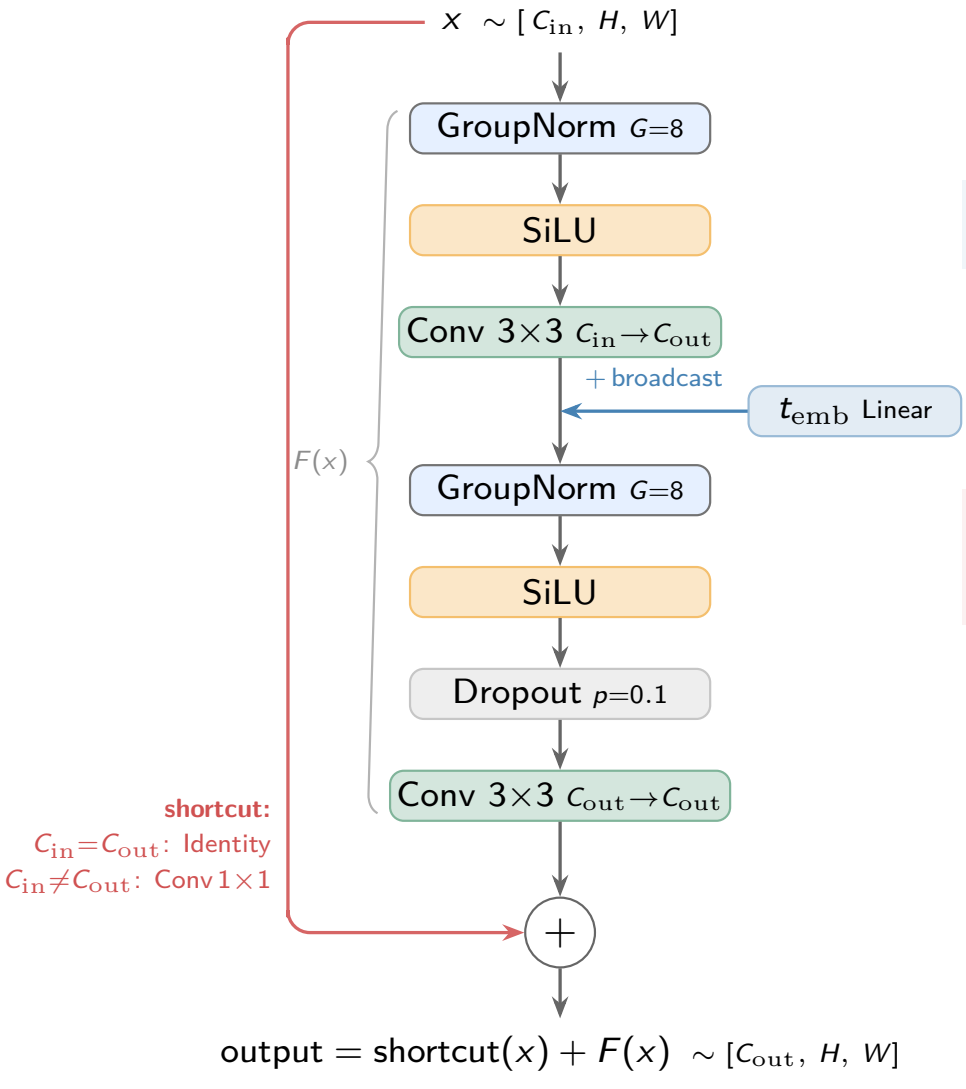
Applied only at 8×8 and 4×4 resolution. Every spatial position attends to every other position, giving the network a global receptive field at low resolution. At higher resolutions, convolutions alone handle local structure.

Time conditioning

The integer timestep t is mapped to a 256-dim vector via sinusoidal positional encoding (log-spaced frequencies), then processed by a 2-layer MLP (Linear → SiLU → Linear). The resulting t_{emb} is broadcast-added to the hidden activations inside every ResBlock (bias-only FiLM: scale = 1, shift = t_{emb}).

Stage	Spatial	Ch	Res	Attn	Notes
Input proj	32^2	$3 \to 64$	–	–	Conv 3×3, padding 1
Enc 0	32^2	64	2		$\downarrow$ Conv stride 2 $\to$ 16^2
Enc 1	16^2	128	2		$\downarrow$ Conv stride 2 $\to$ 8^2
Enc 2	8^2	256	2	✓	$\downarrow$ Conv stride 2 $\to$ 4^2
Enc 3	4^2	512	2	✓	skip saved before $\downarrow$
Bottleneck	4^2	512	2	✓	Res $\to$ SelfAttn $\to$ Res
Dec 0	4^2	512	3	✓	cat skip: $1024 \to 512$
Dec 1	8^2	256	3	✓	$\uparrow$ ConvTranspose stride 2; cat skip
Dec 2	16^2	128	3		$\uparrow$ ConvTranspose stride 2; cat skip
Dec 3	32^2	64	3		$\uparrow$ ConvTranspose stride 2; cat skip
Output	32^2	$64 \to 3$	–	–	GroupNorm $\to$ SiLU $\to$ Conv 3×3

ResBlock: residual block with time conditioning



Layer	Details
GroupNorm	G=8 groups
SiLU	$x \cdot \sigma(x)$; aka swish
Conv2d 3×3	$C_{\text{in}} \to C_{\text{out}}$, padding 1
t_{emb} inject	Linear(d, C_{out}) add to each spatial position $H \times W$
GroupNorm	G=8 groups
SiLU	
Dropout	p=0.1
Conv2d 3×3	$C_{\text{out}} \to C_{\text{out}}$, padding 1
shortcut	$C_{\text{in}} = C_{\text{out}}$: **nn.Identity()** $C_{\text{in}} \neq C_{\text{out}}$: **Conv2d** 1×1 — channel projection only
+	elementwise add: $F(x) + \text{shortcut}(x)$

Design rationale:

- **Pre-activation order** (Norm→Act→Conv): gradients bypass nonlinearities via the shortcut.
- **Time after first conv**: before GroupNorm it would be normalized away.
- **GroupNorm** not BatchNorm: works at batch 1 (sampling).
- 1×1 **shortcut**: channel projection only, no spatial mixing.

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Diffusion avoids the need to balance terms, and the loss decreases monotonically with more training.

Summary

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Component	**Formula / Description**	**Purpose**
Forward process	$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\,\boldsymbol{\epsilon}$	Generate training pairs
Training objective	$\mathbb{E}\big[\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2\big]$	Learn to denoise
Score relation	$s_t(\mathbf{x}_t) = -\frac{\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)}{\sqrt{1-\bar{\alpha}_t}}$	Noise $\leftrightarrow$ score
Reverse mean	$\mu_\theta = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta\right)$	Drift toward data
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The key insights:

- Smoothing makes score learning tractable (Vincent's theorem)
- Noise prediction parameterizes the score field
- Score matching and likelihood maximization (ELBO, appendix) give the same objective
- Sampling follows the learned score field via the reverse process

Questions?

Next: Stable Diffusion

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Why did it take 15 years for score matching to become a generative modeling breakthrough?

The Foundation (2005–2011)

Hyvärinen (2005): Score matching for energy-based models

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What was missing: Multi-scale noise, sampling procedure, deep architectures, generative framing

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3. **Deep learning maturity**
   - U-Nets (2015), ResNets (2016), attention mechanisms (2017)
   - Architectures that could represent complex score fields at multiple scales

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The breakthrough: Combine multi-scale noise with annealed Langevin sampling

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Limitation: trained separate networks for each noise level (inefficient).

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Result: diffusion became the dominant paradigm for image generation.

Appendix: The ELBO Derivation (Full)

This appendix contains the full derivation of the ELBO for diffusion models, referenced in the main lecture.

We show that maximizing the ELBO (evidence lower bound) leads to the same training objective $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\|^2$ derived from score matching.

Roadmap:

1. Write the ELBO in terms of the forward and reverse chains
2. Rearrange it into a sum of KL divergences, one per timestep
3. Compute the forward posterior $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$
4. Show that matching means requires predicting noise
5. Conclude: the ELBO objective is exactly $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\|^2$

See Lecture 21 for background on the ELBO and variational inference.

Roadmap: Validating the Objective via the ELBO

We already derived $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\|^2$ from score matching. What can we say about the likelihood of samples generated from score matching? By connecting score matching to a latent variable model and using the ELBO, we can validate the performance of score matching.

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The derivation is long but each piece is straightforward. We will pause twice to recap progress.

A Second Perspective: The ELBO

Step 1/5: Write ELBO

We have already derived the training objective $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2$ from score matching. Now we ask: does this same objective have a *likelihood-based* justification?

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In Lecture 21 we saw the ELBO—a lower bound on $\log p_\theta(\mathbf{x})$ for any latent variable model:

$$\log p_\theta(\mathbf{x}) \;\geq\; \mathcal{L}_{\text{ELBO}} \;=\; \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}\left[\log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\mathbf{x})}\right].$$

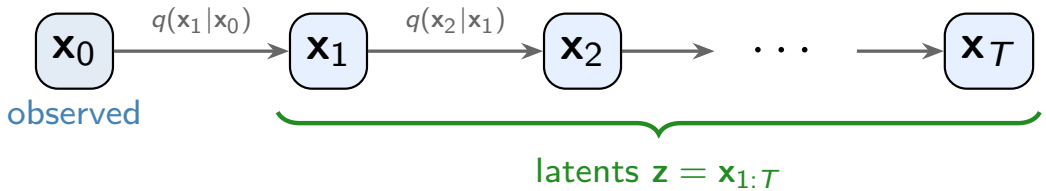
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Diffusion models *are* latent variable models: the latent variables are the entire noisy chain $\mathbf{z} = \mathbf{x}_{1:T}$.



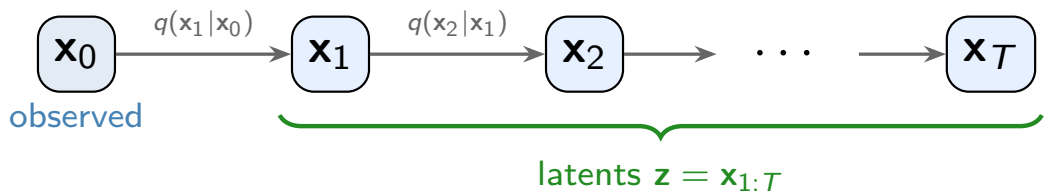
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The forward process $q(\mathbf{x}_{1:T}|\mathbf{x}_0)$ is the approximate posterior (fixed, not learned). We still need to specify the reverse $p_\theta(\mathbf{x}_{0:T})$—a *design decision*.

Writing Out the ELBO for Diffusion

Substituting $\mathbf{z} = \mathbf{x}_{1:T}$ into the ELBO:

$$\mathcal{L}_{\text{ELBO}} = \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right].$$

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For the reverse, we *choose* to model p_θ as a Markov chain running backward from pure noise: $p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$. This is a **design choice**: our generative model reverses the chain one step at a time. We have not yet specified the *form* of each $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$.

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With both factorizations, the log-ratio inside the expectation becomes

$$\log p(\mathbf{x}_T) + \sum_{t=1}^{T} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}.$$

The Rearrangement Problem

We need to rearrange the sum

$$\log p(\mathbf{x}_T) + \sum_{t=1}^{T} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}$$

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The difficulty: the ratio $\frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}$ compares two distributions that condition on *different* variables. The numerator conditions on $\mathbf{x}_t$ and produces $\mathbf{x}_{t-1}$; the denominator conditions on $\mathbf{x}_{t-1}$ and produces $\mathbf{x}_t$.

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The tool for flipping conditionals is Bayes' rule.

Applying Bayes' Rule to the Forward Process

Recall Bayes' rule for conditional distributions: given random variables A, B, C,

$$q(A \mid B, C)\, q(B \mid C) = q(B \mid A, C)\, q(A \mid C).$$

This is just the chain rule for probability applied twice.

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Set $A = \mathbf{x}_t$, $B = \mathbf{x}_{t-1}$, $C = \mathbf{x}_0$. Then:

$$q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0)\, q(\mathbf{x}_{t-1} \mid \mathbf{x}_0) = q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)\, q(\mathbf{x}_t \mid \mathbf{x}_0).$$

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By the Markov property of the forward process, $\mathbf{x}_t$ depends on $\mathbf{x}_{t-1}$ alone, so $q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0) = q(\mathbf{x}_t \mid \mathbf{x}_{t-1})$.

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Solving for $q(\mathbf{x}_t|\mathbf{x}_{t-1})$:

$$\boxed{q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\; q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}.}$$

Substituting into the Log-Ratio Sum

Replace each $q(\mathbf{x}_t|\mathbf{x}_{t-1})$ in the denominator:

$$\sum_{t=1}^{T} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}$$

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Split the log of the product into a sum of logs:

$$= \underbrace{\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{\text{reconstruction } (t=1)} + \sum_{t=2}^{T} \Bigg[\underbrace{\log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)}}_{\text{compares reverse distributions}} + \underbrace{\log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)}}_{\text{ratio of forward marginals}}$$

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The first piece (for $t \geq 2$) compares $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ to $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$—both are distributions over $\mathbf{x}_{t-1}$ conditioned on $\mathbf{x}_t$—exactly what we wanted.

The Telescoping Sum

The t=1 term in the first piece is the **reconstruction term** $\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)$, pulled out separately. For $t \geq 2$, write out the forward-marginal ratios:

$$t = 2: \quad \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{q(\mathbf{x}_2|\mathbf{x}_0)}$$

$$t = 3: \quad \log \frac{q(\mathbf{x}_2|\mathbf{x}_0)}{q(\mathbf{x}_3|\mathbf{x}_0)}$$

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Each numerator cancels the denominator of the next term. After cancellation only the last denominator survives:

$$\sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} \;=\; \log q(\mathbf{x}_1|\mathbf{x}_0) - \log q(\mathbf{x}_T|\mathbf{x}_0).$$

Assembling the ELBO

Collecting everything, pulling out the $t{=}1$ term (reconstruction), and recognizing KL divergences:

$$\mathcal{L}_{\text{ELBO}} = \underbrace{-D_{\mathrm{KL}}\big(q(\mathbf{x}_T|\mathbf{x}_0) \,\|\, p(\mathbf{x}_T)\big)}_{\text{prior matching}}$$

$$- \sum_{t=2}^{T} \underbrace{D_{\mathrm{KL}}\big(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \,\|\, p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)\big)}_{\mathcal{L}_t\text{: denoising matching at step } t}$$

$$+ \underbrace{\mathbb{E}_q[\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)]}_{\text{reconstruction}}$$

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(Minus signs because we *maximize* the ELBO; training *minimizes* $-\mathcal{L}_{\text{ELBO}}$, i.e. minimizes the KL terms.)

Assembling the ELBO

Collecting everything, pulling out the $t{=}1$ term (reconstruction), and recognizing KL divergences:

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Each $\mathcal{L}_t$ compares the learned reverse $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ against the forward posterior $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ we just computed.

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We choose $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{0}, \mathbf{I})$ as our prior—pure isotropic noise. From the one-shot formula, $q(\mathbf{x}_T|\mathbf{x}_0) = \mathcal{N}\big(\sqrt{\bar{\alpha}_T}\,\mathbf{x}_0,\ (1-\bar{\alpha}_T)\mathbf{I}\big)$.

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We *design* the noise schedule so that $\bar{\alpha}_T \approx 0$, which means $\sqrt{\bar{\alpha}_T} \approx 0$ and $\sqrt{1-\bar{\alpha}_T} \approx 1$. Then $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{0}, \mathbf{I}) = p(\mathbf{x}_T)$, so this KL is ≈ 0.

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This measures how well the model recovers the clean data $\mathbf{x}_0$ from the almost-clean $\mathbf{x}_1$. Since the first noise step β_1 is very small, $\mathbf{x}_1 \approx \mathbf{x}_0$, and this term is typically small.

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The real work happens in the $\sum_{t=2}^{T} \mathcal{L}_t$ terms.

Checkpoint: ELBO Decomposition Complete

Steps 1–2 of 5 complete

Where we are in the roadmap:

- ✓ Write the ELBO in terms of the forward and reverse chains
- ✓ Rearrange it into a sum of KL divergences, one per timestep
- ☐ Figure out what distribution the reverse process should match at each step
- ☐ Show that matching means requires predicting noise
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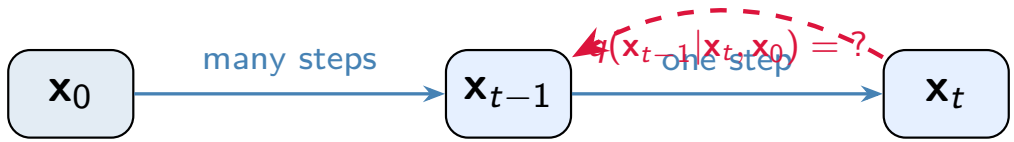
To answer that, we first need to know what $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ is.

Why Condition on $\mathbf{x}_0$?

The KL terms involve $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$—the forward process conditioned on *both* $\mathbf{x}_t$ *and* the original clean data $\mathbf{x}_0$. Why?

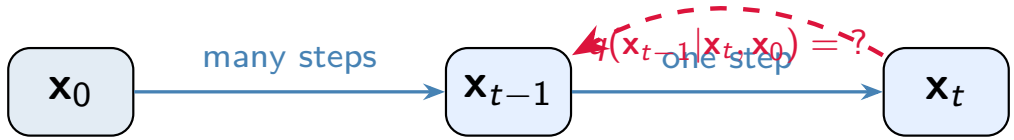
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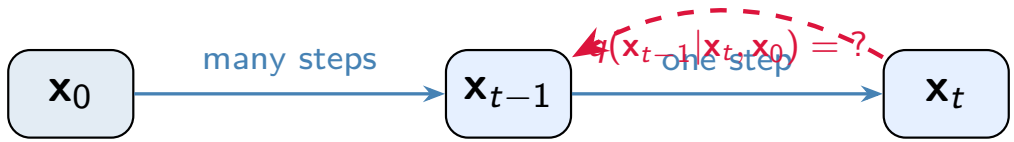
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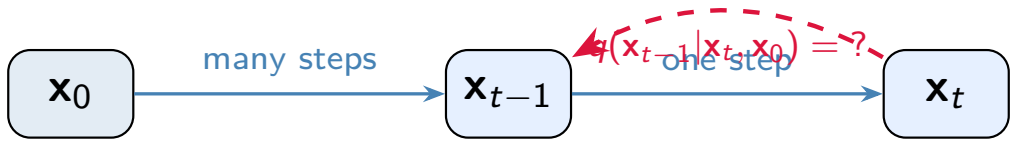


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Both $q(\mathbf{x}_{t-1}|\mathbf{x}_0)$ and $q(\mathbf{x}_t|\mathbf{x}_{t-1})$ are Gaussian, so $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ is also Gaussian with a closed-form formula.

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We call $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ the **forward posterior** at step t: *posterior* because it updates our belief about $\mathbf{x}_{t-1}$ after observing $\mathbf{x}_t$ and $\mathbf{x}_0$; *forward* because it uses only the forward process q (no learned parameters).

Gaussian Conditioning Theorem

To compute $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$, we use a standard fact about multivariate Gaussians.

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Theorem (Conditioning in a Joint Gaussian)

If $\mathbf{y}$ and $\mathbf{z}$ are jointly Gaussian (given some fixed conditioning variable),

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu}_y \\ \boldsymbol{\mu}_z \end{pmatrix}, \begin{pmatrix} \Sigma_{yy} & \Sigma_{yz} \\ \Sigma_{zy} & \Sigma_{zz} \end{pmatrix} \right),$$

then the conditional distribution of $\mathbf{y}$ given $\mathbf{z}$ is

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We will apply this with $\mathbf{y} = \mathbf{x}_{t-1}$ and $\mathbf{z} = \mathbf{x}_t$, both conditioned on $\mathbf{x}_0$. So we need the joint distribution $(\mathbf{x}_{t-1}, \mathbf{x}_t \mid \mathbf{x}_0)$: its mean vector and its 2×2 covariance matrix.

The Joint Distribution $(\mathbf{x}_{t-1}, \mathbf{x}_t \mid \mathbf{x}_0)$

From the forward process, both marginals conditioned on $\mathbf{x}_0$ are Gaussian. Writing d for the dimension of $\mathbf{x}$:

Means (from the one-shot formula):

$$\mathbb{E}[\mathbf{x}_{t-1} \mid \mathbf{x}_0] = \sqrt{\bar{\alpha}_{t-1}}\,\mathbf{x}_0, \qquad \mathbb{E}[\mathbf{x}_t \mid \mathbf{x}_0] = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0.$$

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Marginal variances: $\mathrm{Var}(\mathbf{x}_{t-1} \mid \mathbf{x}_0) = (1 - \bar{\alpha}_{t-1})\,\mathbf{I}$, $\mathrm{Var}(\mathbf{x}_t \mid \mathbf{x}_0) = (1 - \bar{\alpha}_t)\,\mathbf{I}$.

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Cross-covariance: Since $\mathbf{x}_t = \sqrt{\alpha_t}\,\mathbf{x}_{t-1} + \sqrt{\beta_t}\,\boldsymbol{\epsilon}_t$ with $\boldsymbol{\epsilon}_t$ independent of $\mathbf{x}_{t-1}$,

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All blocks of the joint covariance matrix are proportional to $\mathbf{I}$, so the conditioning theorem reduces to scalar formulas applied coordinate-wise.

Computing the Posterior Variance

Step 3/5: Compute forward posterior

Apply the conditioning theorem with $\mathbf{y} = \mathbf{x}_{t-1}$, $\mathbf{z} = \mathbf{x}_t$. Since all covariance blocks are proportional to $\mathbf{I}$, we work with scalars.

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To simplify the bracket, use $\bar{\alpha}_t = \alpha_t\bar{\alpha}_{t-1}$, so

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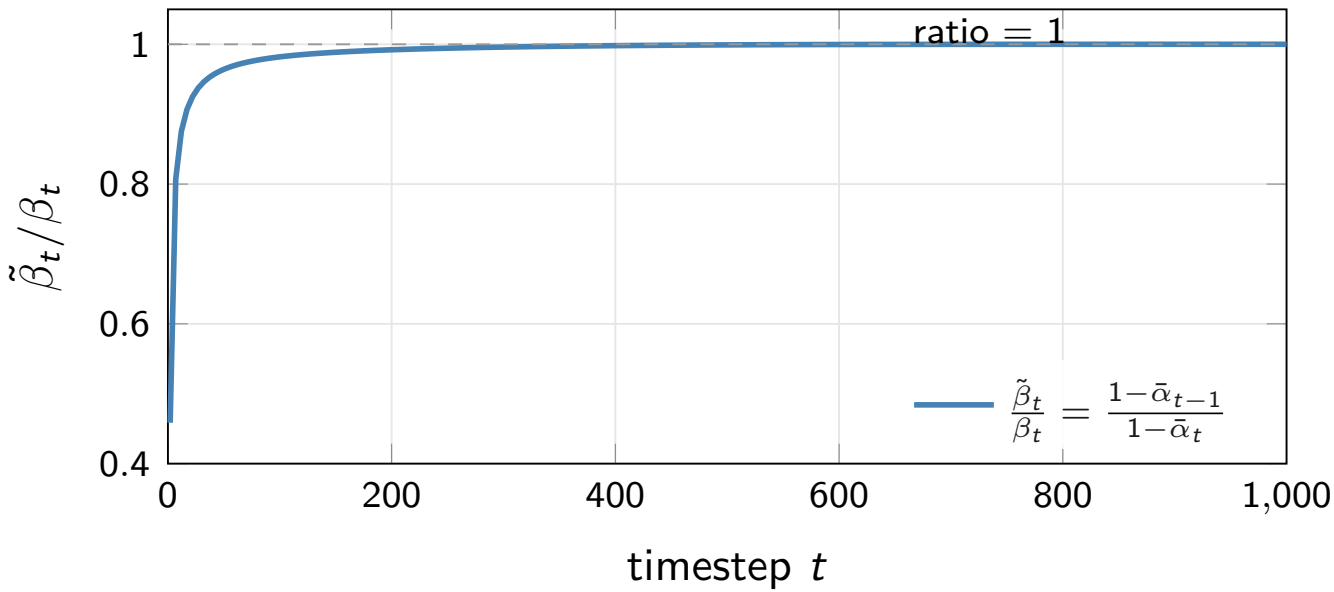
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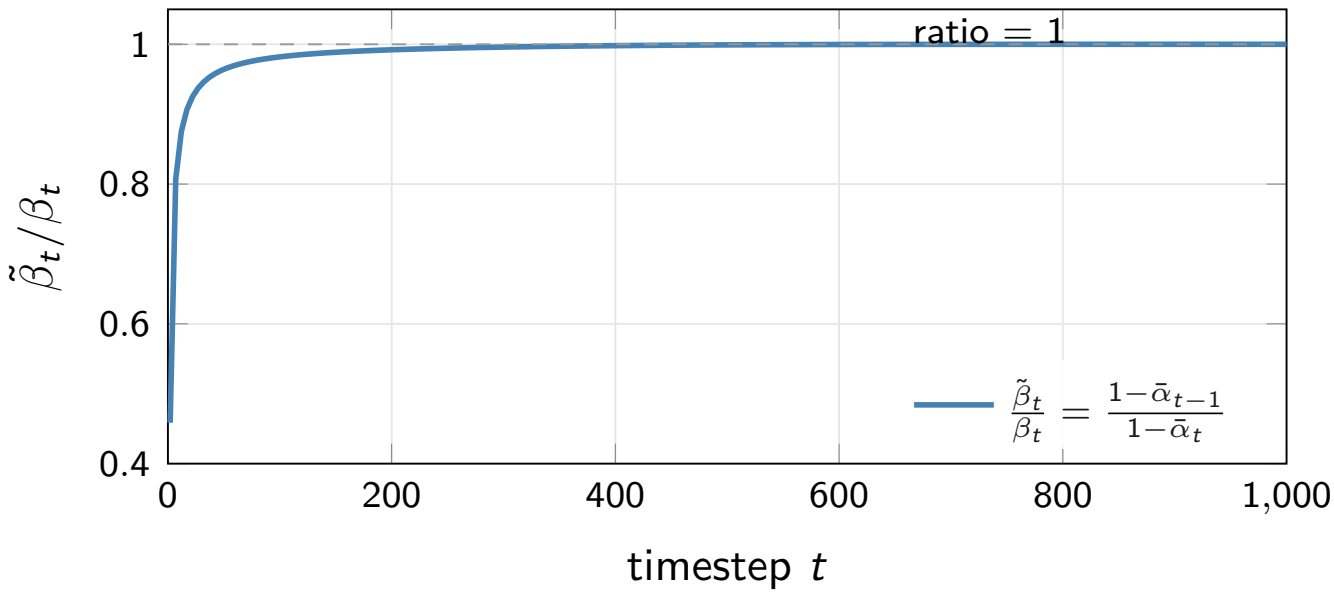
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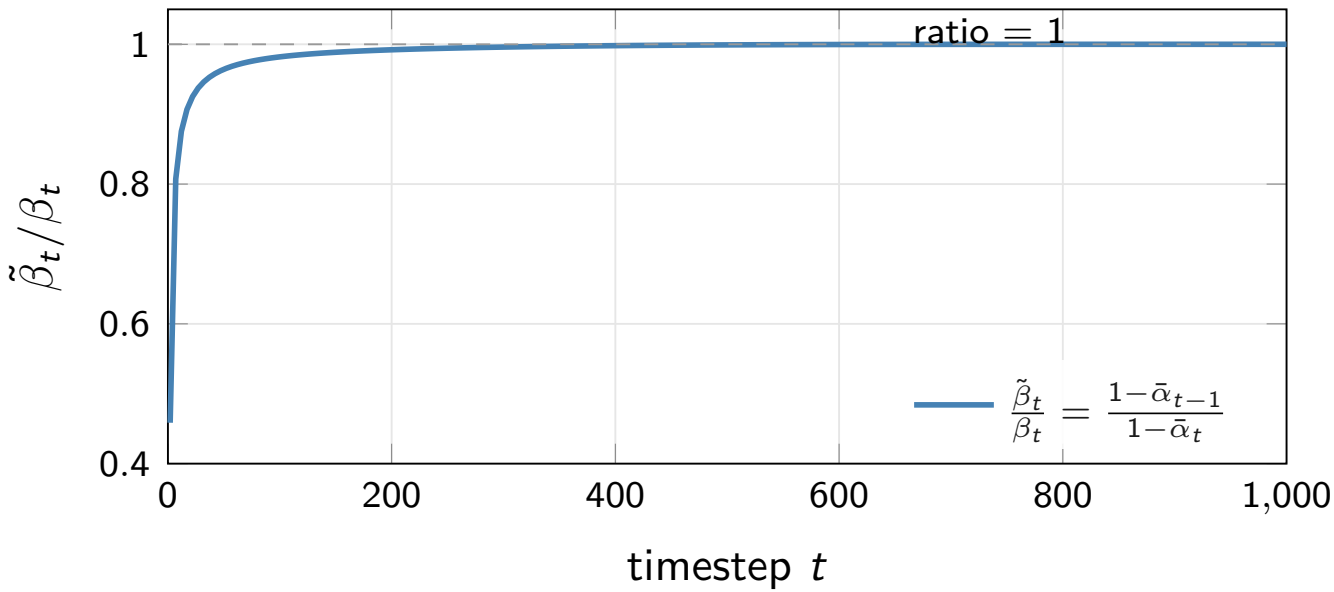


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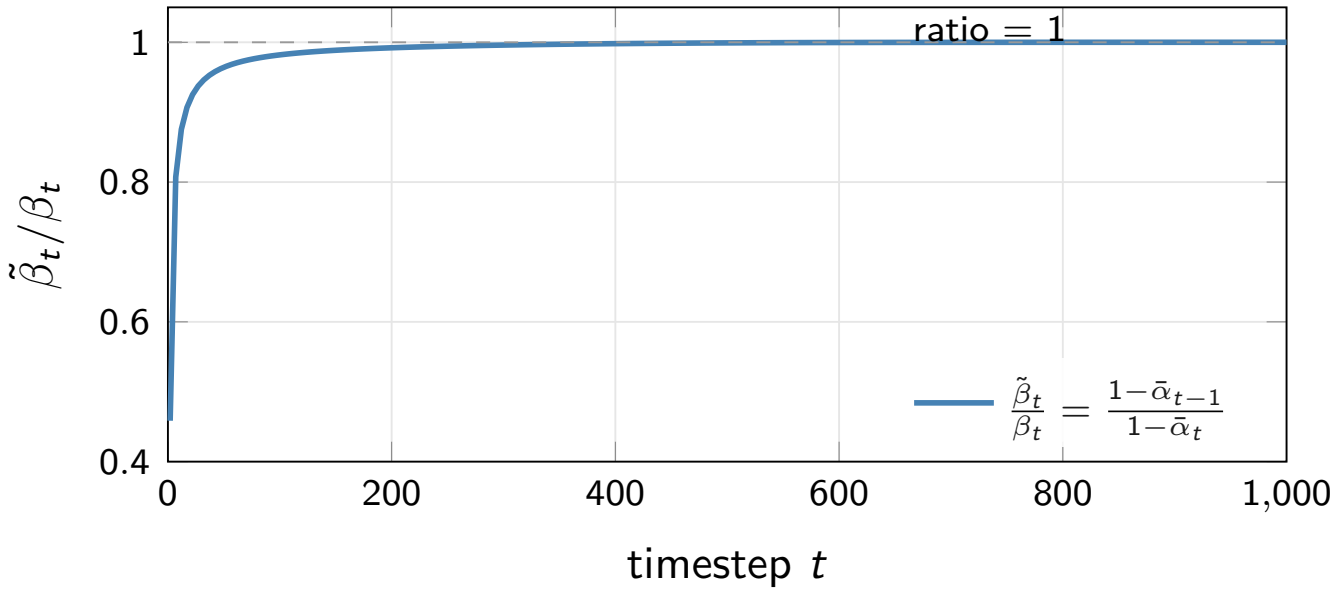


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- At large t: ratio ≈ 1 — conditioning on $\mathbf{x}_t$ provides little extra information

Why Is the Posterior Variance Smaller?

Geometric intuition: When t is small and there's little noise, knowing *both* $\mathbf{x}_t$ and $\mathbf{x}_0$ pins down $\mathbf{x}_{t-1}$ more tightly than knowing just $\mathbf{x}_0$ alone—hence $\tilde{\beta}_t < \beta_t$.

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At small t, the two are highly correlated (one forward step apart), so conditioning reduces variance significantly. At large t, both are dominated by independent noise, so little correlation to exploit.

Computing the Posterior Mean

Posterior mean. Define $\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$ as the mean vector (the conditioning theorem gives us $\boldsymbol{\mu}_y + \Sigma_{yz}\Sigma_{zz}^{-1}(\mathbf{z} - \boldsymbol{\mu}_z)$):

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Expand and collect the $\mathbf{x}_0$ terms. The coefficient of $\mathbf{x}_0$ is:

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Final result:

$$\boxed{\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\bar{\alpha}_{t-1}}\,\beta_t}{1-\bar{\alpha}_t}\,\mathbf{x}_0 \;+\; \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\,\mathbf{x}_t.}$$

Interpreting the Forward Posterior

Putting the pieces together:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}\big(\mathbf{x}_{t-1};\ \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0),\ \tilde{\beta}_t\, \mathbf{I}\big).$$

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Formula	$\dfrac{\sqrt{\bar{\alpha}_{t-1}}\,\beta_t}{1-\bar{\alpha}_t}$	$\dfrac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}$
Large t (high noise)	small	large
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This makes intuitive sense: when there is little noise (t small), $\mathbf{x}_t \approx \mathbf{x}_0$ already and the posterior trusts $\mathbf{x}_0$ heavily. When noise is high (t large), $\mathbf{x}_t$ carries less information about $\mathbf{x}_0$, so the posterior relies more on $\mathbf{x}_t$ itself.

Checkpoint: We Know What to Match

Step 3 of 5 complete

Where we are in the roadmap:

- ✓ Write the ELBO in terms of the forward and reverse chains
- ✓ Rearrange it into a sum of KL divergences, one per timestep
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What we just computed: The distribution we need to match is

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where $\tilde{\mu}_t$ and $\tilde{\beta}_t$ have closed-form expressions in terms of the noise schedule.

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What's left: Choose a parameterization for $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ and show that minimizing $D_{\mathrm{KL}}\big(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\,\|\,p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)\big)$ is equivalent to predicting the noise ϵ.

Choosing a Form for p_θ: Two Design Decisions

We now need to specify the form of $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$. Nothing in the ELBO derivation forces a particular choice—this is where we make **modeling decisions**.

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With these choices, the ELBO's KL terms compare two Gaussians with the same variance:

Forward posterior (known given $\mathbf{x}_0$)

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}\big(\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0),\ \tilde{\beta}_t \mathbf{I}\big)$$

$\mathcal{L}_t = D_{\mathrm{KL}}$

Learned reverse (our design choice)

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}\big(\mu_\theta(\mathbf{x}_t, t),\ \tilde{\beta}_t \mathbf{I}\big)$$

KL Between Gaussians with Matched Variance

When two Gaussians share the same covariance Σ, their KL divergence reduces to a squared Mahalanobis distance between their means:

$$D_{\mathrm{KL}}\big(\mathcal{N}(\mu_1, \Sigma) \,\|\, \mathcal{N}(\mu_2, \Sigma)\big) = \tfrac{1}{2}(\mu_1 - \mu_2)^\top \Sigma^{-1}(\mu_1 - \mu_2).$$

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Applying this to $\mathcal{L}_t$ with $\Sigma = \tilde{\beta}_t \, \mathbf{I}$:

$$\mathcal{L}_t = \frac{1}{2\tilde{\beta}_t} \left\| \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_\theta(\mathbf{x}_t, t) \right\|^2 .$$

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Training the reverse process reduces to making its predicted mean $\mu_\theta(\mathbf{x}_t, t)$ match the true reverse mean $\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$.

From Mean Matching to Noise Prediction

Step 5/5: Parameterize via ϵ_θ

We want $\mu_\theta(\mathbf{x}_t, t) \approx \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$.

From Mean Matching to Noise Prediction

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The true mean is $\mathbf{x}_t$ corrected by $\boldsymbol{\epsilon}$. We already have $\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)$ (from score matching) to predict it, so we parameterize:

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\,\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right).$$

The KL Reduces to Noise Prediction

Substituting $\tilde{\mu}_t$ and μ_θ into the matched-variance KL formula from two slides ago, the $\mathbf{x}_t$ terms cancel (both means have the same $\mathbf{x}_t/\sqrt{\alpha_t}$ component), leaving:

$$\mathcal{L}_t = \frac{\beta_t^2}{2\tilde{\beta}_t\,\alpha_t(1-\bar{\alpha}_t)}\,\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2\,.$$

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The weight $w_t = \frac{\beta_t^2}{2\tilde{\beta}_t\,\alpha_t(1-\bar{\alpha}_t)}$ depends only on the noise schedule—it varies with t but has no learnable parameters.

The Simplified Objective

Summing over all timesteps, the ELBO loss is a weighted sum of noise-prediction errors:

$$-\mathcal{L}_{\text{ELBO}} = \sum_{t=2}^{T} w_t \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right\|^2 + (\text{prior} + \text{reconstruction}),$$

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Ho et al. (2020) found empirically that *dropping the weights* w_t and using the unweighted objective

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t,\, \mathbf{x}_0,\, \boldsymbol{\epsilon}} \left[\left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right\|^2 \right]$$

works better in practice.

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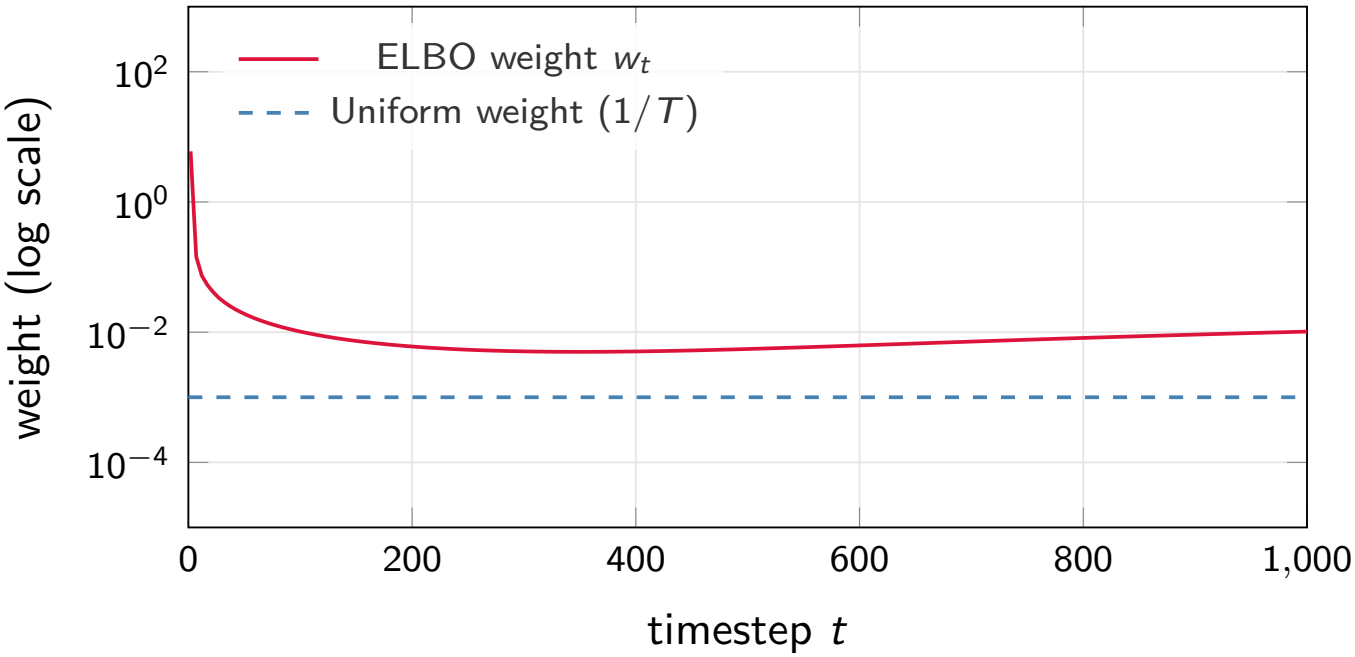
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Why would ignoring the theoretically correct weights help? The next slide visualizes the difference.

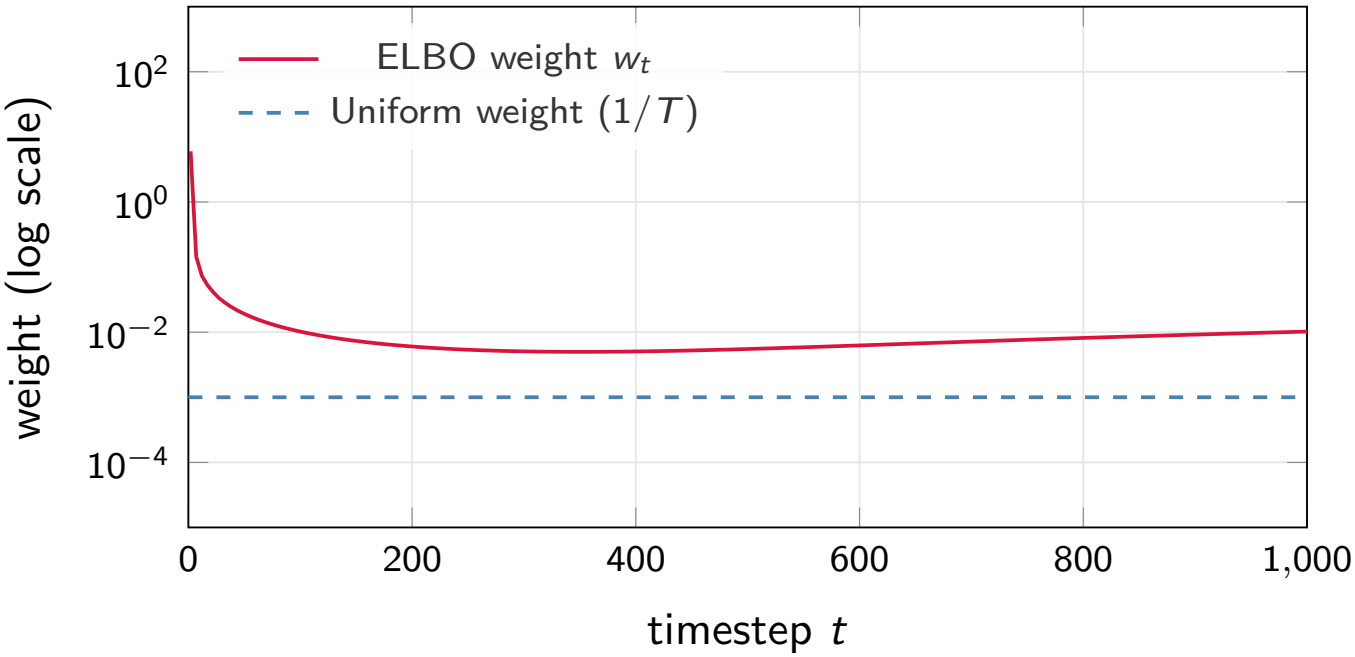
Visualizing ELBO Weights vs. Uniform Weights

Using the linear schedule $\beta_1 = 10^{-4}$, $\beta_T = 0.02$, $T = 1000$:



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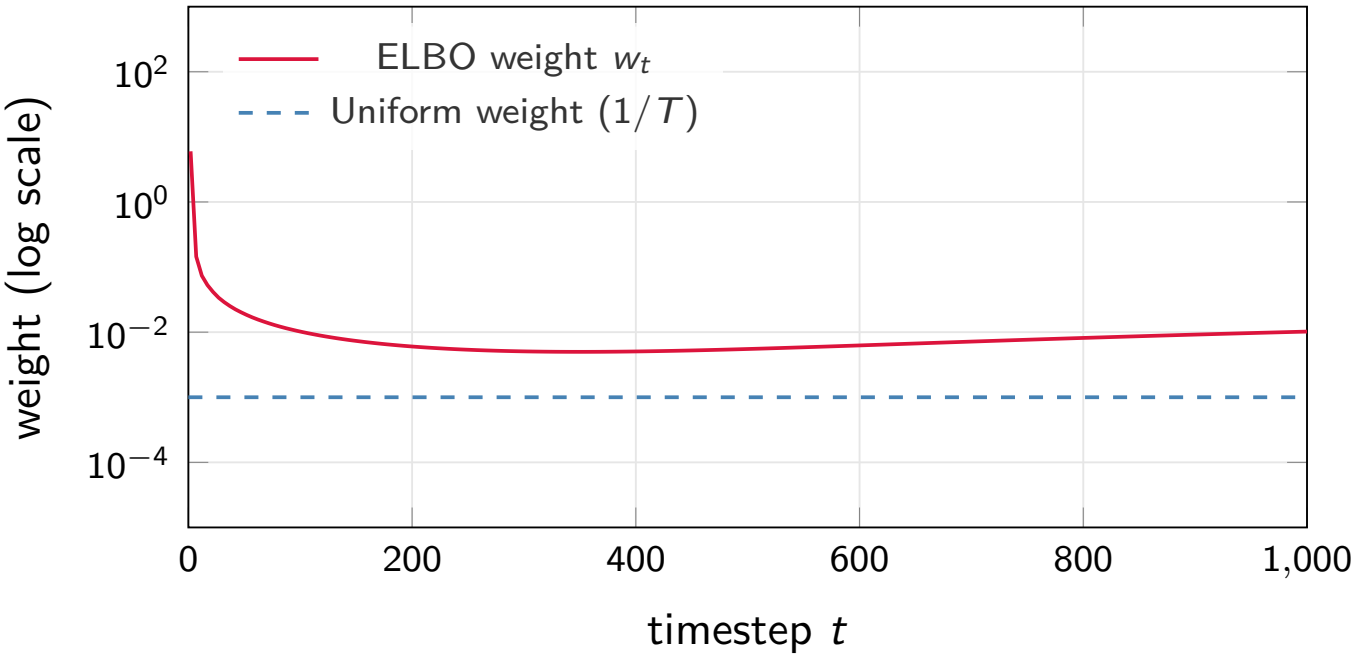
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The ELBO weights w_t grow *exponentially*, reaching over 200 at t=1000. The theoretically correct objective heavily emphasizes high-noise timesteps.

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The ELBO weights w_t grow *exponentially*, reaching over 200 at t=1000. The theoretically correct objective heavily emphasizes high-noise timesteps.

Uniform weighting $(1/T)$ ignores this imbalance. Empirically, Ho et al. found uniform weighting works *better*—learning fine details at low t matters more for sample quality than the ELBO suggests.

Recap: From ELBO to ϵ-Prediction

All 5 steps complete

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The punchline: Maximizing the ELBO is equivalent to minimizing

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t,\, \mathbf{x}_0,\, \boldsymbol{\epsilon}} \left[\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2 \right].$$

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- ✓ Show that matching means requires predicting noise
- ✓ Conclude: the ELBO objective is exactly $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\|^2$

The punchline: Maximizing the ELBO is equivalent to minimizing

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t,\, \mathbf{x}_0,\, \boldsymbol{\epsilon}} \left[\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2 \right].$$

This is exactly what we got from score matching. Two independent derivations, same objective.

Two Roads to the Same Objective

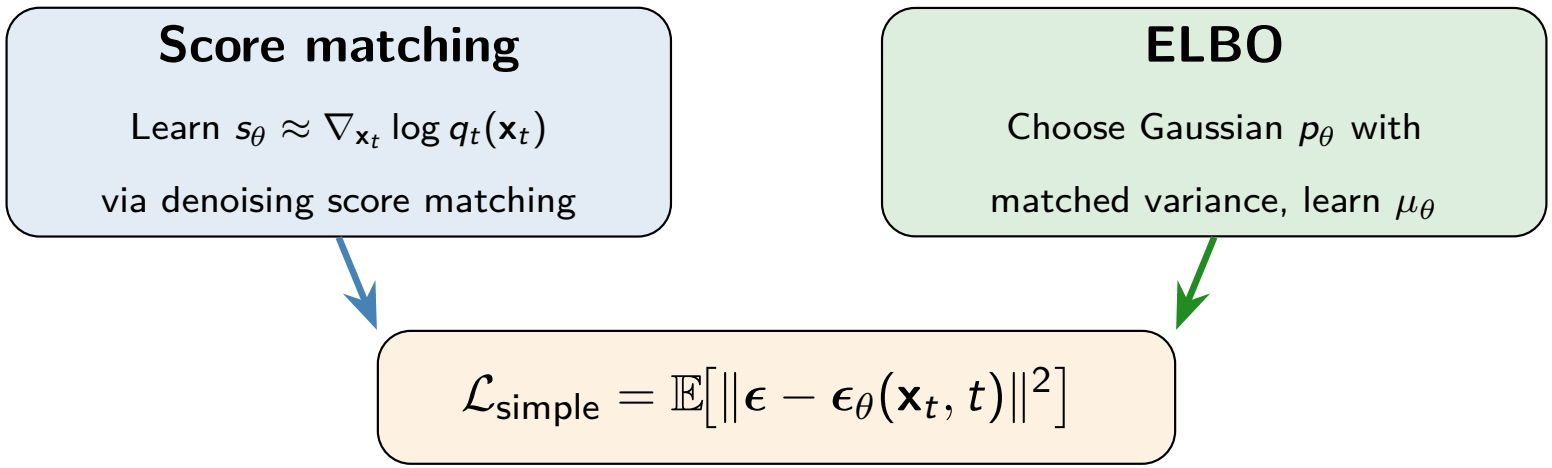
All steps complete

We arrived at $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2$ by two independent routes:

Two Roads to the Same Objective

All steps complete

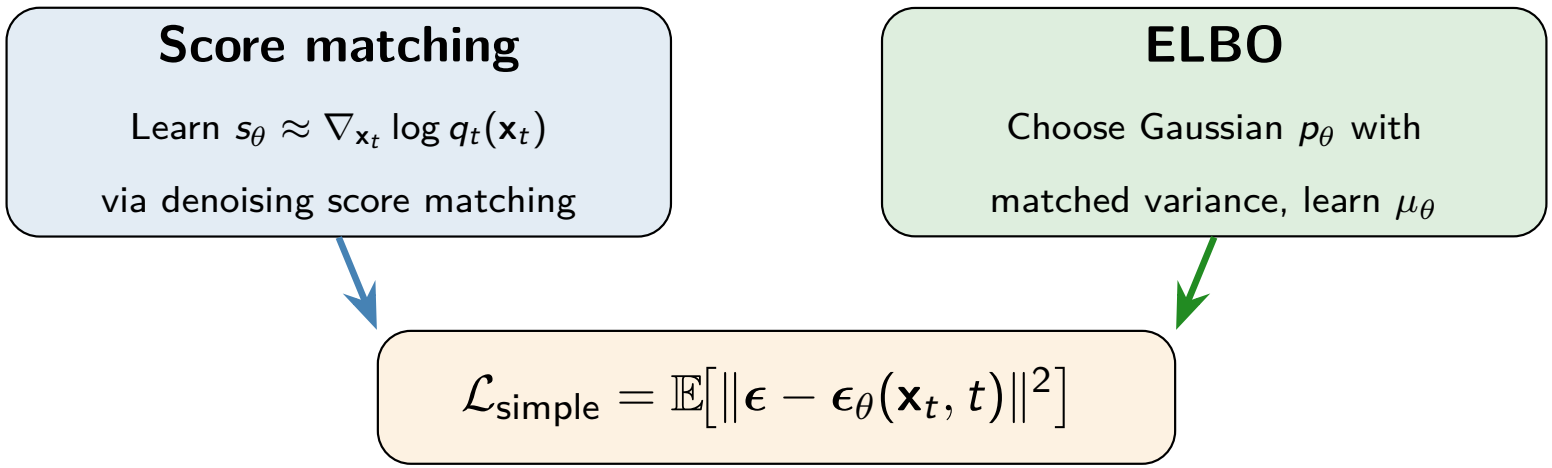
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Two Roads to the Same Objective

All steps complete

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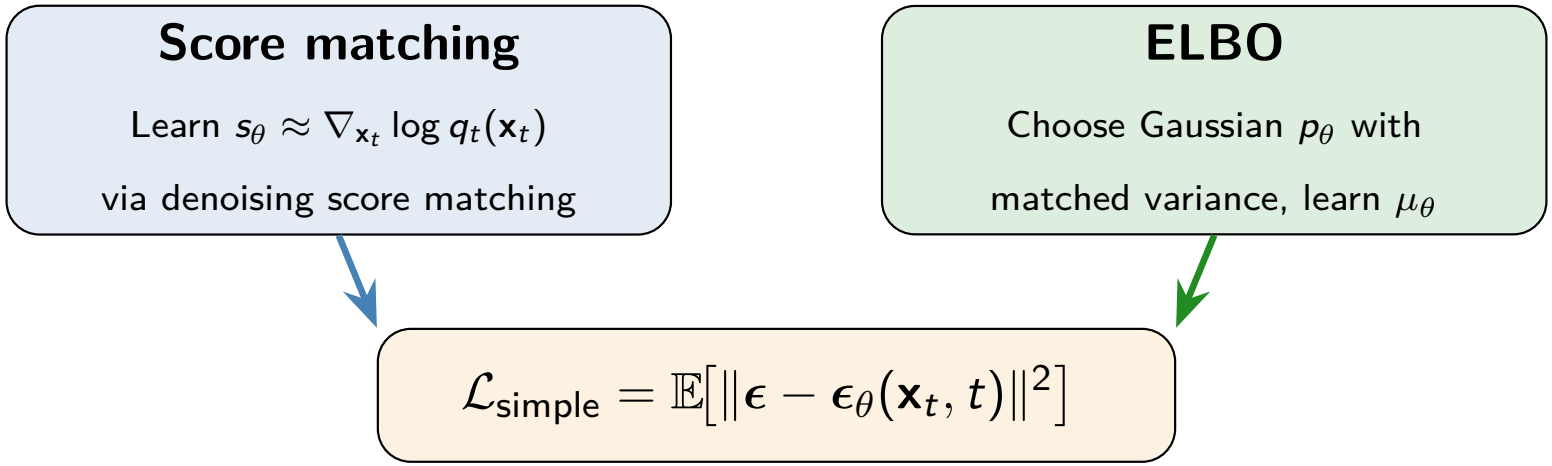


Each route provides a different guarantee about what $\boldsymbol{\epsilon}_\theta$ is doing:

Two Roads to the Same Objective

All steps complete

We arrived at $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2$ by two independent routes:

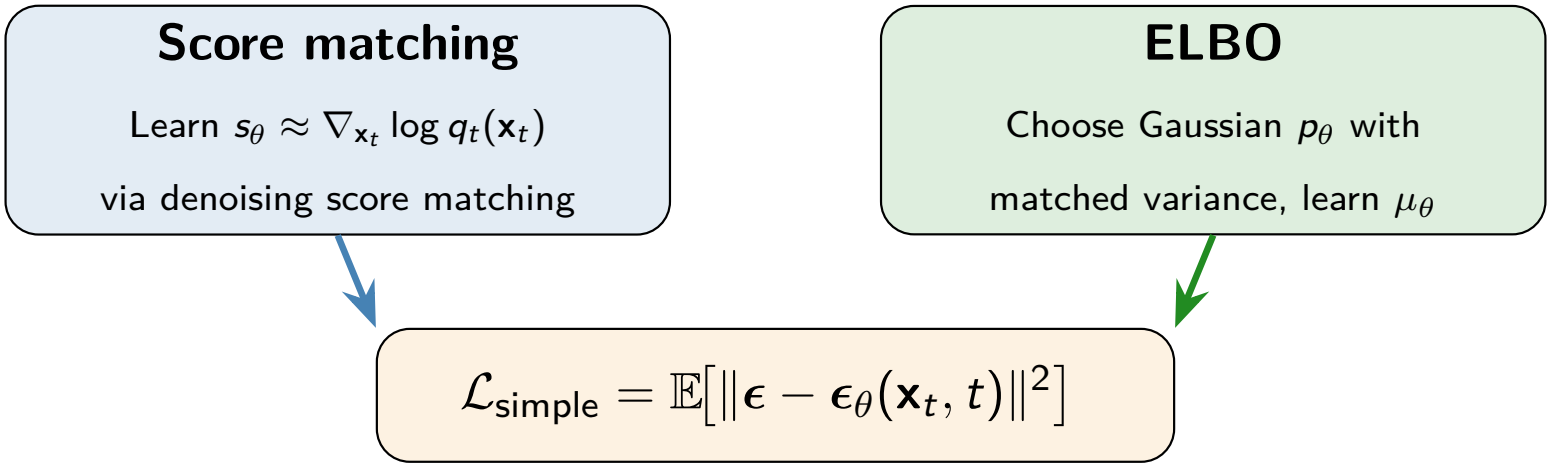


Each route provides a different guarantee about what $\boldsymbol{\epsilon}_\theta$ is doing:

Perspective	**Guarantee**	**Design choices**
Score matching	Learns $\nabla \log q_t$	ϵ-parameterization
ELBO	Maximizes likelihood bound	Gaussian p_θ, matched var.

Two Roads to the Same Objective

We arrived at $\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2$ by two independent routes:



Each route provides a different guarantee about what $\boldsymbol{\epsilon}_\theta$ is doing:

Perspective	**Guarantee**	**Design choices**
Score matching	Learns $\nabla \log q_t$	ϵ-parameterization
ELBO	Maximizes likelihood bound	Gaussian p_θ, matched var.

In practice, use whichever view helps you reason about the problem at hand.