Diffusion Models: Theory

From a known noising process back to data — predict the noise, then reverse it

Prof. Nipun Batra

ES 667 · Deep Learning · IIT Gandhinagar

The generative problem becomes denoising

Why a new family of generative models?

Q QUESTION

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the key move: if we **know** how to add noise, we can train a network to **remove** it

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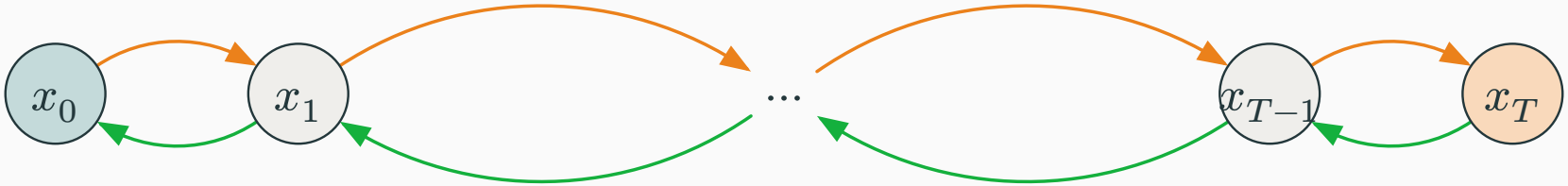

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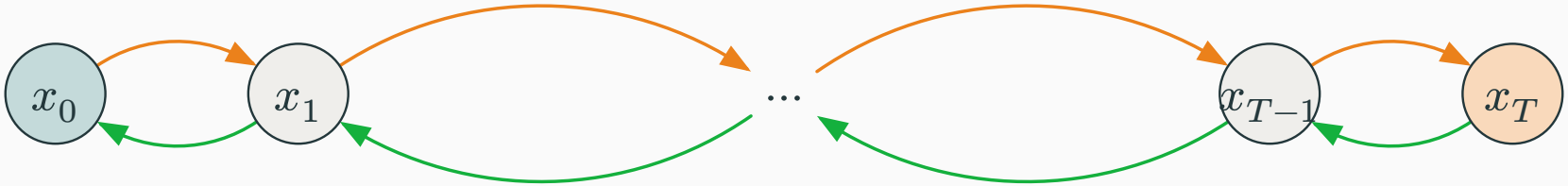

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forward is **fixed and known**; only the **reverse** transitions are **learned**

Visual hook: the noising filmstrip

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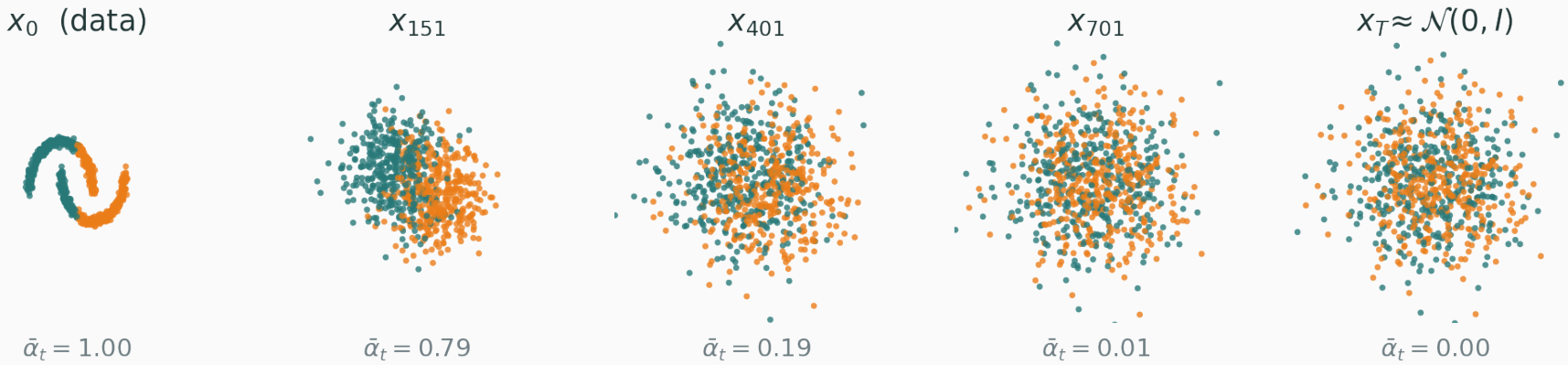

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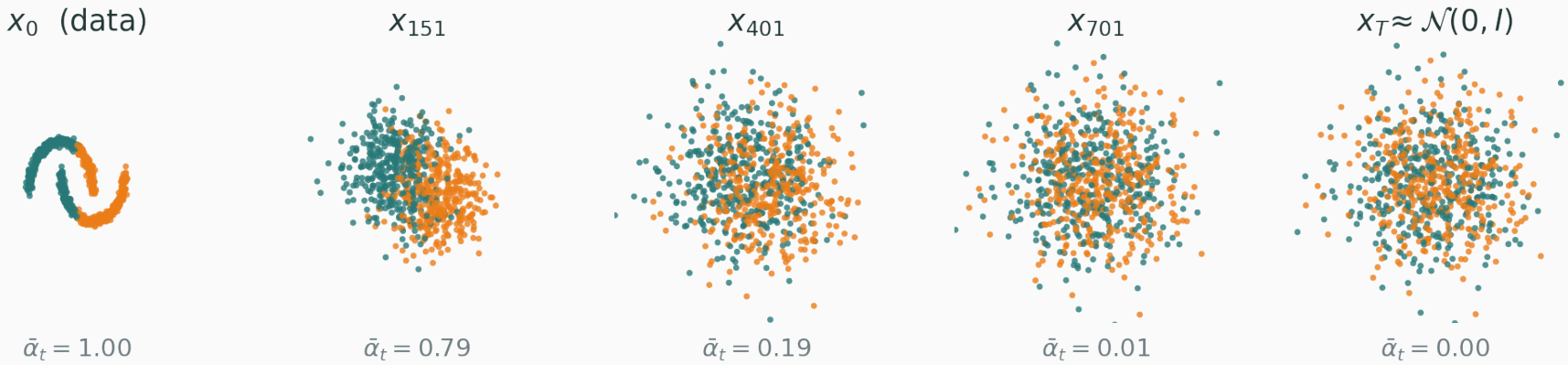

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structure dissolves smoothly; by $t = T$ the sample is **indistinguishable from pure noise**

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$\sqrt{1-\beta_t}$ **scales down** the previous sample; $\beta_t I$ **adds** fresh noise

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$\overline{\alpha}_t$ falls from ≈ 1 (early) toward ≈ 0 (late) — it is the whole story of the schedule

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each step barely changes the sample — many **tiny** steps accumulate into total corruption

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mean $\sqrt{\overline{\alpha}_t}\, x_0$ is the **surviving signal**; variance $(1 - \overline{\alpha}_t) I$ is the **accumulated noise**

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> we **know the noise** because we drew it ourselves — this is the crux of the whole method

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signal $\sqrt{\overline{\alpha}_t}\,x_0 = 0.8$ — most of the clean value survives here

noise $\sqrt{1 - \overline{\alpha}_t}\,\varepsilon = -0.3$ — a moderate perturbation at this t

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so generation can **start from pure noise** and only needs to learn the way **back**

Learning the reverse process

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so we model the reverse step **probabilistically**, and learn it from data

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the network must turn a slightly-noisier x_t into a slightly-cleaner x_{t-1}

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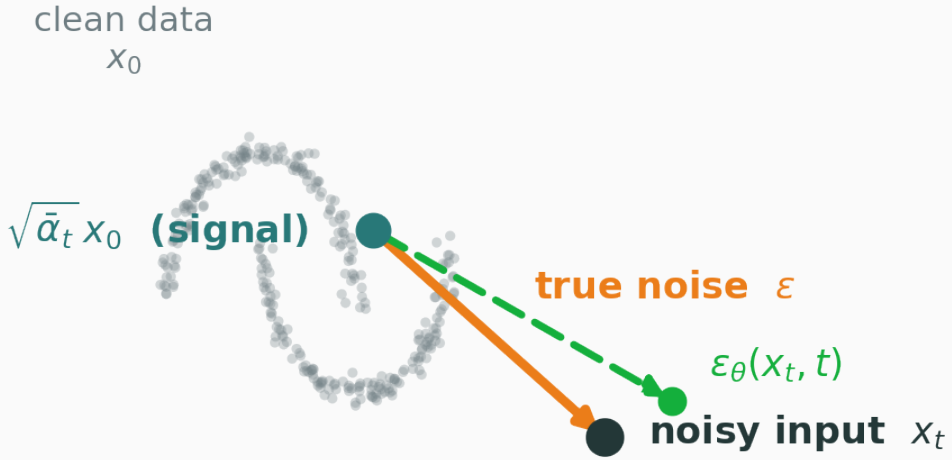
the supervised target is the injected noise; train $\varepsilon_\theta(x_t, t) \approx \varepsilon$



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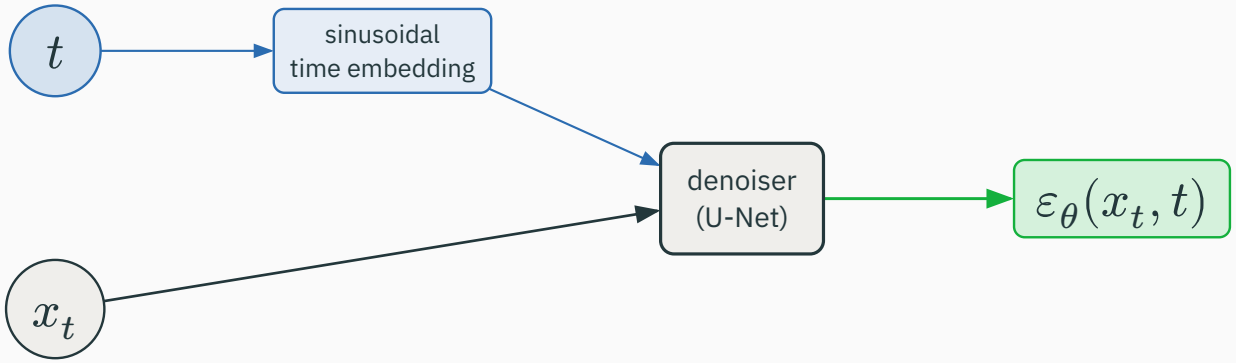

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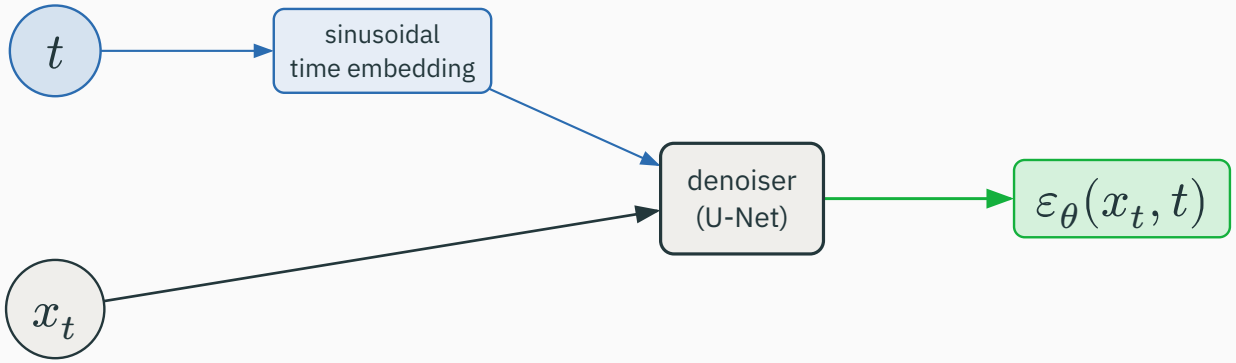

it **must** see t: “remove a little noise” and “remove almost all noise” are different jobs

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the whole of DDPM training is: **sample noise, predict it, minimize the MSE**

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diffusion is denoising self-supervision at **every** noise level at once

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predicting the noise and predicting the clean image are **two views of the same quantity**

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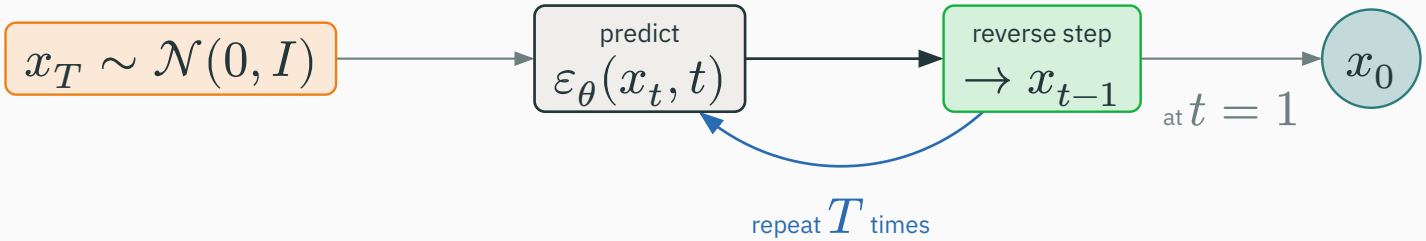

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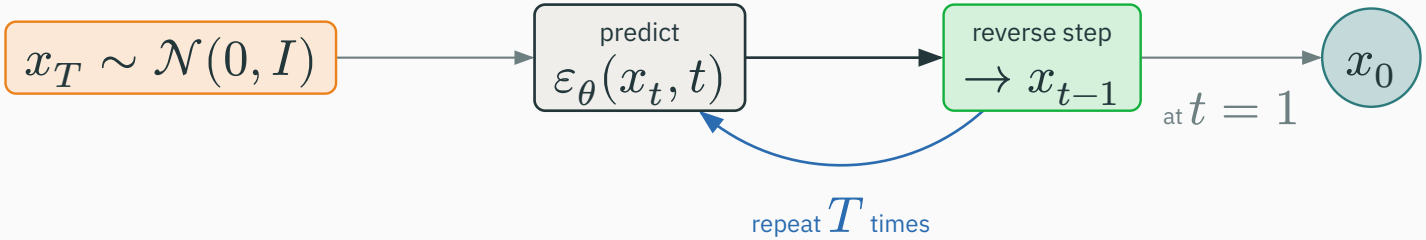


```
x_T ~ N(0, I)                          # start from pure Gaussian noise
for t = T, ..., 1:
    eps_hat = eps_theta(x_t, t)        # predict the noise
    x_{t-1} = reverse_step(x_t, eps_hat, t)   # sample / estimate x_{t-1}
return x_0
```

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The **mean** is just $\hat{x}_0$'s information re-expressed as a small step toward $t-1$; $\sigma_t^2 = \beta_t$ (or the exact posterior variance) sets how much fresh noise to re-inject. Setting $z = 0$ gives the deterministic (DDIM-style) step.

Interactive: forward and reverse

I INTERACTIVE

INTERACTIVE

↗ nipunbatra.github.io/interactive-articles/diffusion-denoise

Slide the noise level to watch $x_t = \sqrt{\bar{\alpha}_t}\, x_0 + \sqrt{1-\bar{\alpha}_t}\, \varepsilon$ corrupt an example, then run the reverse chain step-by-step and see a sample condense out of noise.

Why generation is slow

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Diffusion — the **same** denoiser is called **hundreds to thousands** of times per sample.

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stable training and broad coverage — paid for in **inference** time (L22 attacks this)

Interpreting the geometry

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- **early** reverse steps (near pure noise) — recover **global layout** and coarse structure;
- **late** reverse steps (nearly clean) — restore **fine texture** and detail.

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one network, but the **job changes** along the trajectory — hence the time conditioning

The noise schedule is a curriculum

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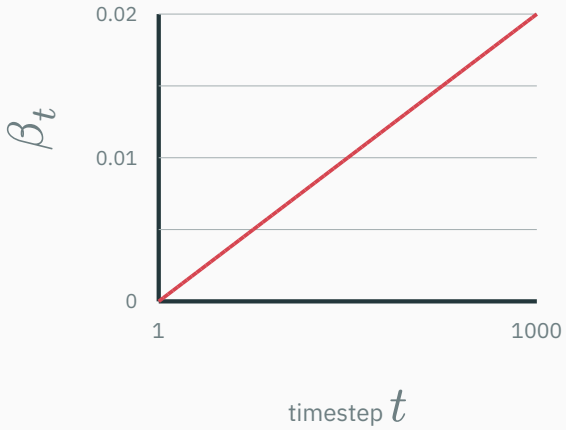
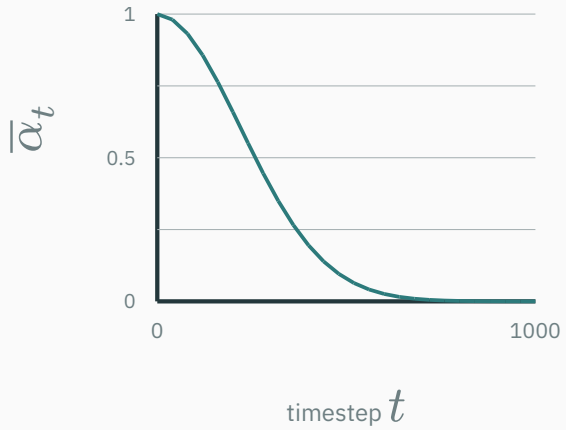
β_t: $10^{-4} \rightarrow 0.02$ **(linear)**



$\overline{\alpha}_t$: **signal retained**



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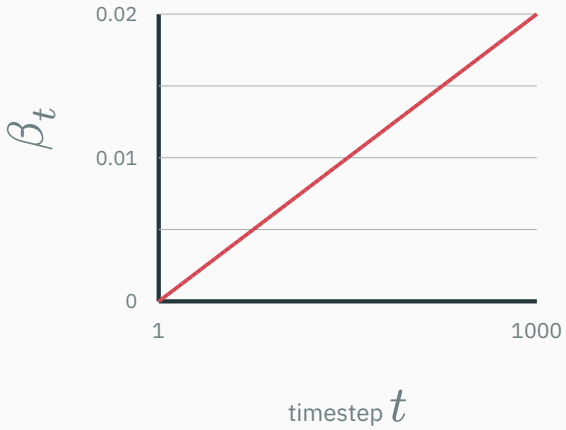

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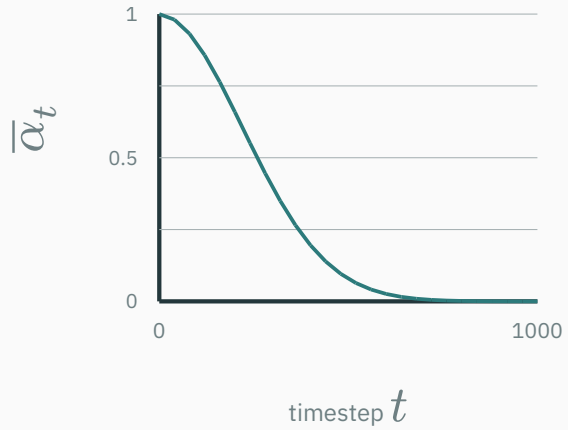

β_t (how much noise each step adds) sets $\overline{\alpha}_t$ (how much signal survives)

The score connection — one conceptual slide

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a bridge to **score-based** models — we stop here, no SDE derivation

What the network actually learns

Q QUESTION

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it learns, from any noisy point, a local direction toward where the data density is high

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a **vector field of denoising directions** — generalized across inputs, timesteps, and conditions

Conditional generation, previewed

D DERIVATION

Feed the denoiser extra information c so the trajectory follows a desired target:

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the denoising **question** is unchanged — only the **conditioning** differs (full story in L22)

Three generative families so far

V VISUAL

Family	Training signal	Sampling
VAE	likelihood (ELBO) bound	one latent decode
GAN	adversarial critic	one generator pass
Diffusion	predict **known** injected noise	repeated denoising

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diffusion trades a **hard sampler** for an **easy, stable** learning signal

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the central trade of the method: **training ease** against **sampling cost**

Knowledge check

Q QUESTION

If t is **large** (a very noisy input), should the model rely more on the **noisy input** or on its **learned data prior**? Why?

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At large t, x_t carries **almost no signal** ($\overline{\alpha}_t \approx 0$). The denoiser must lean on the **prior** it learned — the input mostly tells it **which** broad direction, not the fine details.

Closing bridge to practice

D DERIVATION

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L22 answers all three

Diffusion theory in depth

The forward chain factorizes

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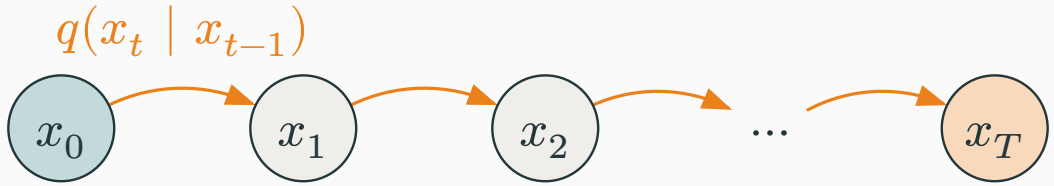

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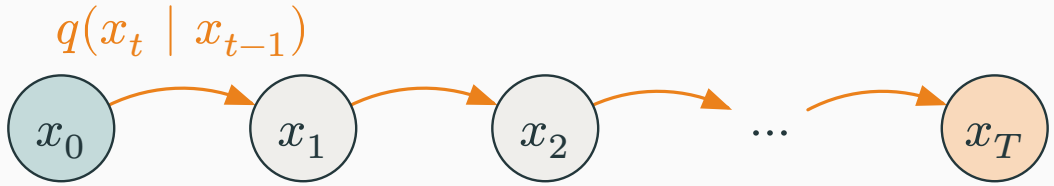

a simple, fixed structure — even when the data distribution is wildly complicated

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Sampling runs the learned chain from the easy prior downward:

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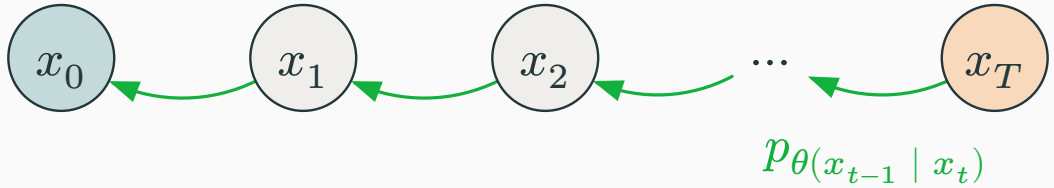

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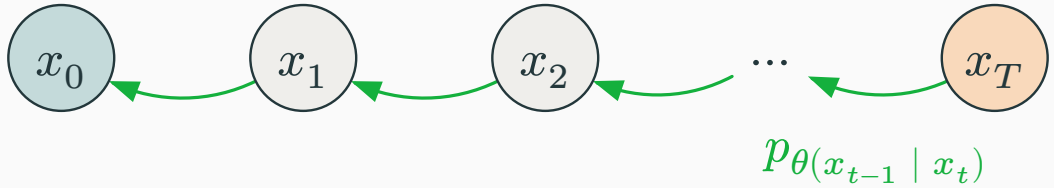

start at $\mathcal{N}(0, I)$, apply T learned reverse transitions, arrive at x_0

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D DERIVATION

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naive — to get x_t, simulate $x_1 \to x_2 \to \ldots \to x_t$. Costly, and different for every t.

closed form — $x_t = \sqrt{\overline{\alpha}_t}x_0 + \sqrt{1-\overline{\alpha}_t}\varepsilon$ in **one** operation, for **any** t.

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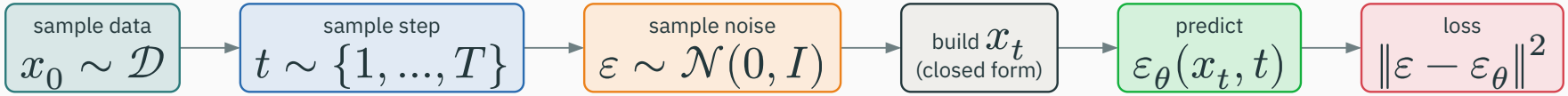
one random t gives one training example in a **single** step — this is what makes training feasible

Training touches every noise difficulty

V VISUAL



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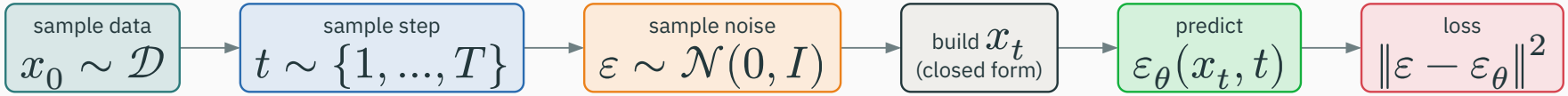

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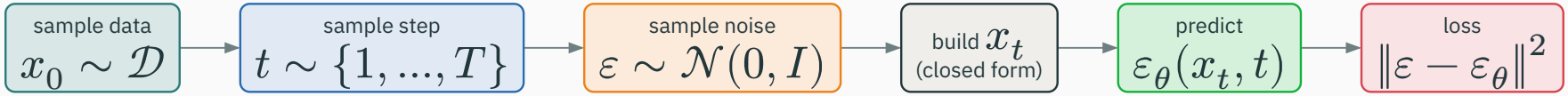

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sample x_0 $\longrightarrow$ sample t $\longrightarrow$ sample ε $\longrightarrow$ build x_t $\longrightarrow$ predict $\varepsilon_{\theta(x_t,t)}$

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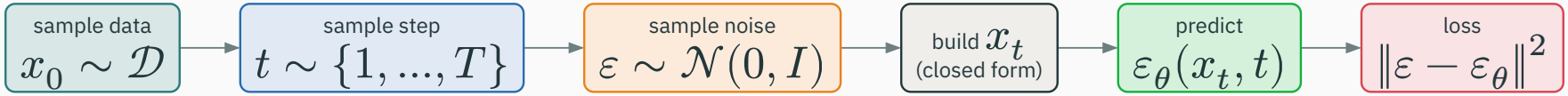

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the same data point spawns a **continuum** of self-supervised denoising tasks

Reading the noise schedule

V VISUAL

Plot the signal and noise coefficients against t:

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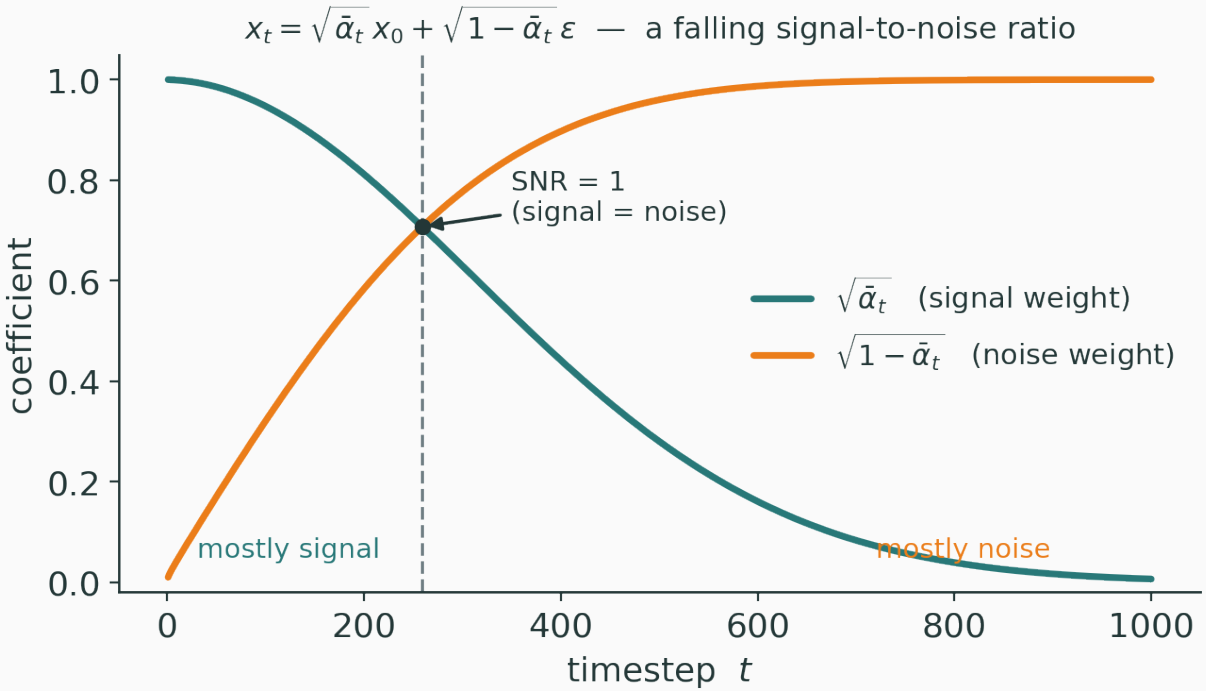

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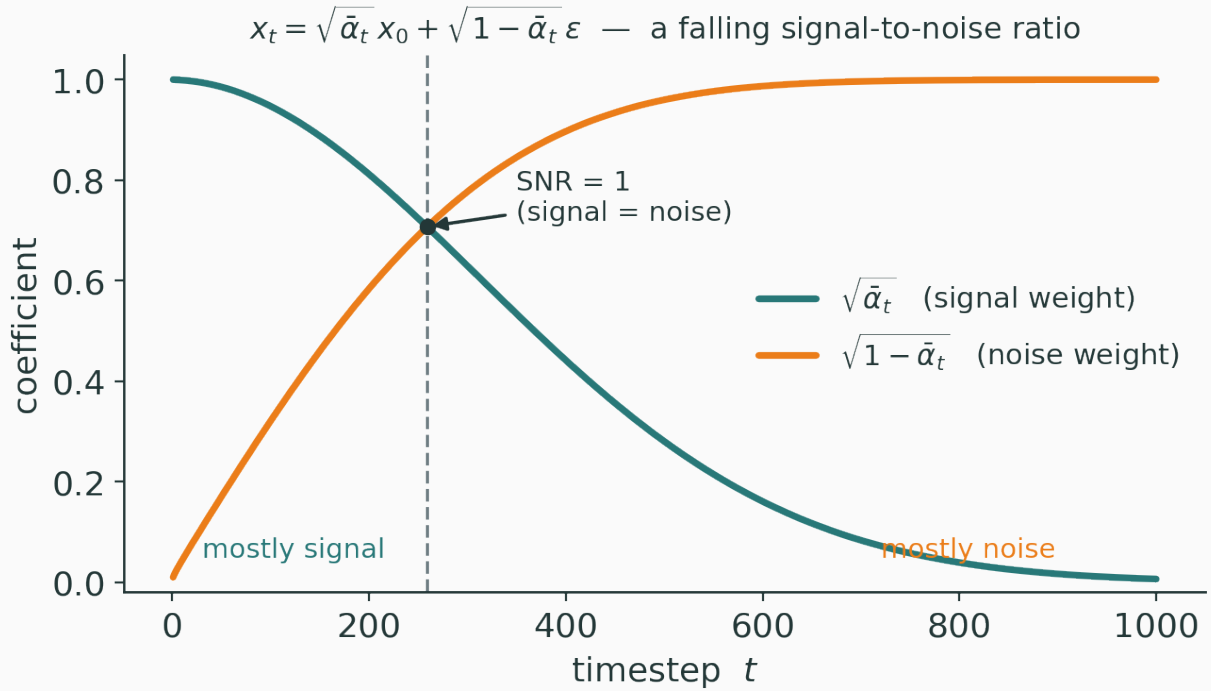

$\sqrt{\bar{\alpha}_t}$ falls from 1; $\sqrt{1-\bar{\alpha}_t}$ rises to 1 — a steadily **falling signal-to-noise ratio**

Different timesteps are different tasks

V VISUAL

Timestep	Input appearance	Main denoising demand
small t	mostly clean	remove fine perturbations
middle t	partly structured	recover objects / layout
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the time embedding tells the network **which** of these regimes it is in

Why predict noise rather than the image?

D DERIVATION

Several equivalent parameterizations exist:

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the parameterization is a **modeling choice**, not the essence of diffusion

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Minimizing MSE makes ε_θ approach the **conditional mean** of the noise given x_t. It blends the evidence in x_t with the **data prior** — exactly what a good denoiser should do.

Time must enter the network

V VISUAL

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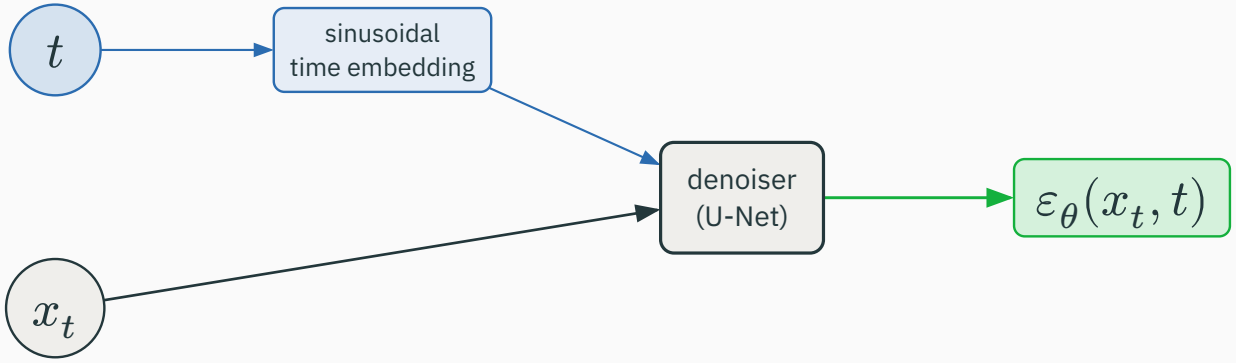

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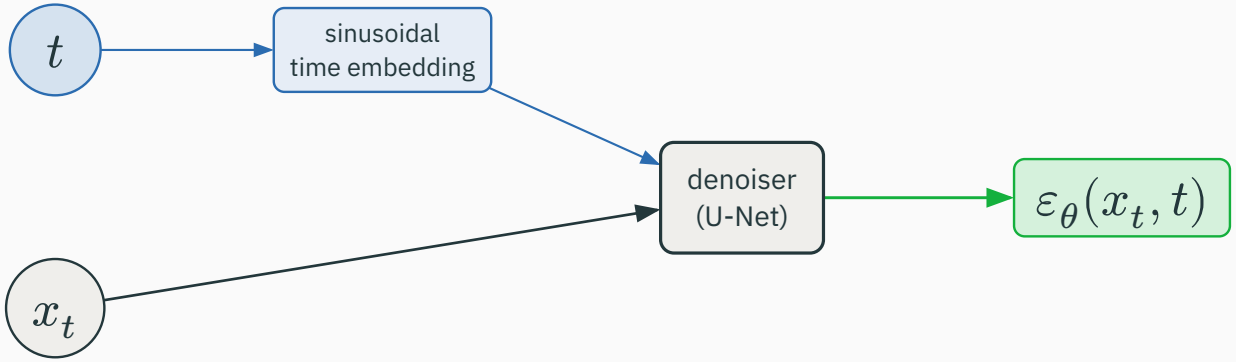

$t \longrightarrow$ sinusoidal / learned embedding $\longrightarrow$ injected into the denoiser blocks

Reverse-mean intuition

V VISUAL

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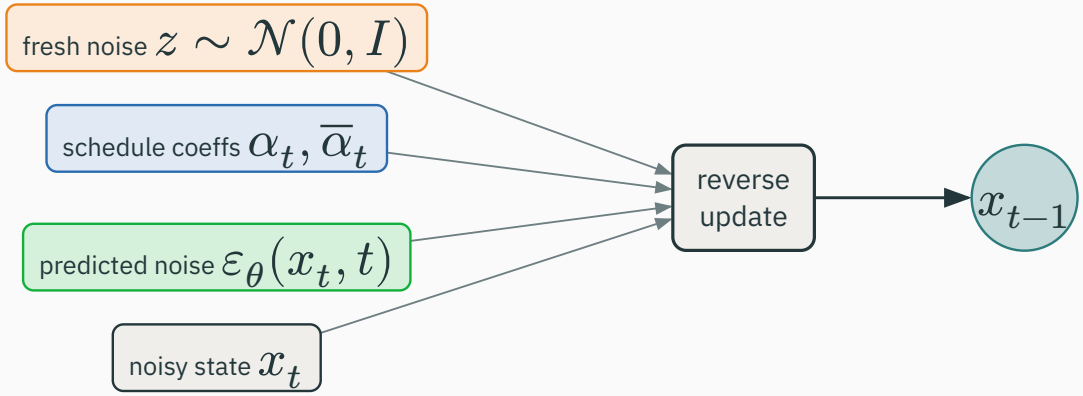

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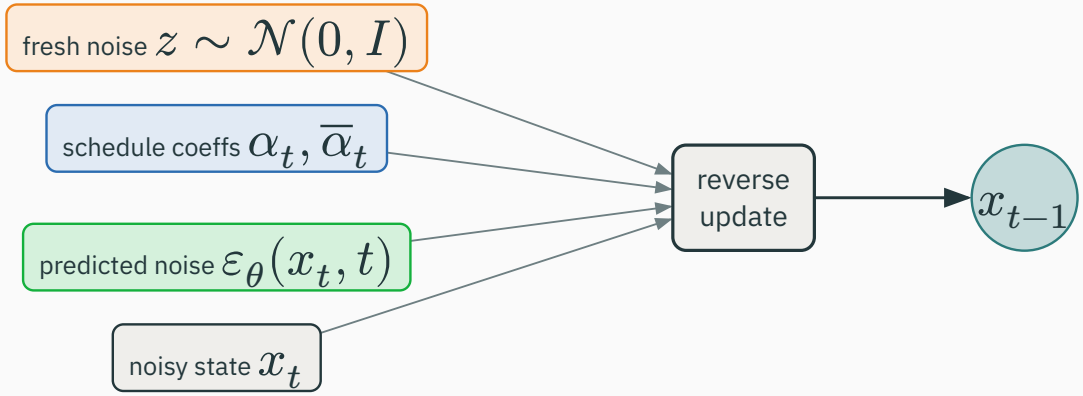

current state, predicted noise, schedule, and (optionally) fresh randomness $\longrightarrow x_{t-1}$

Stochastic vs deterministic sampling

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this changes diversity, reproducibility, and speed — **not** the learned denoiser itself

One sample, many intermediate states

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Run the reverse chain and watch a value settle onto a data mode:

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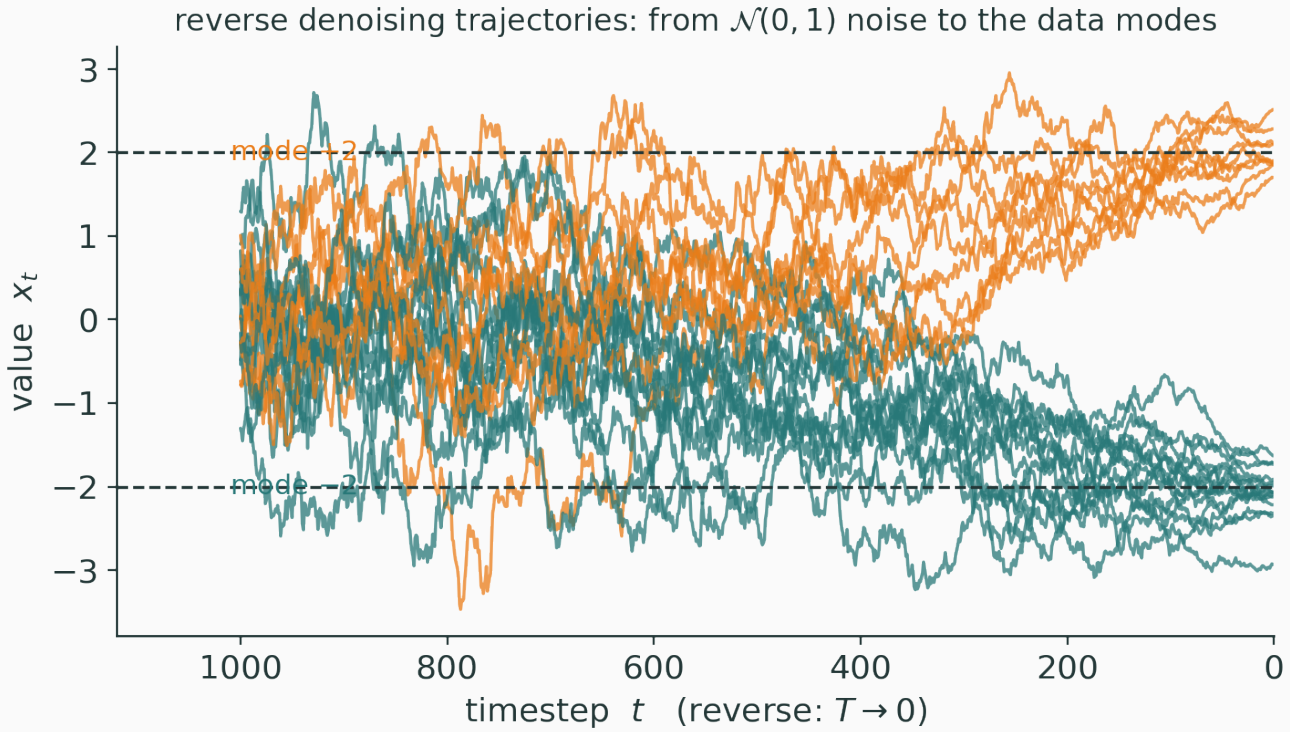

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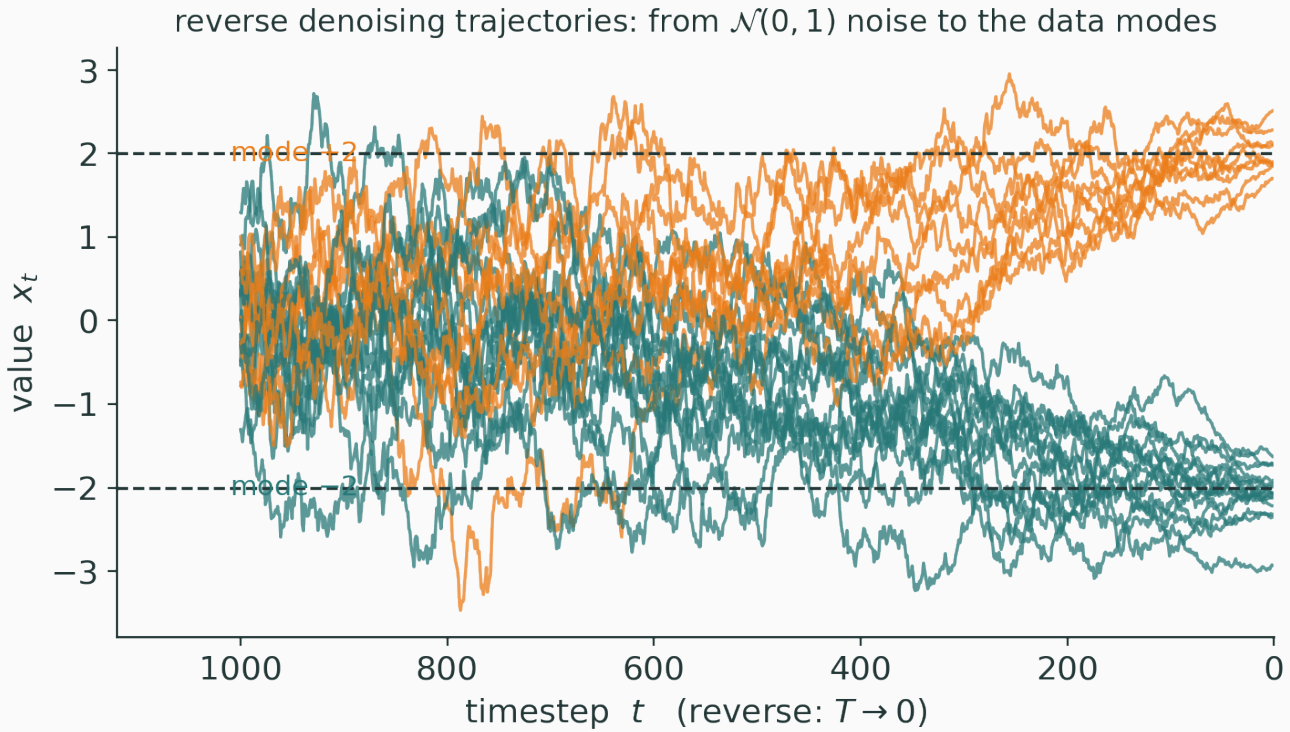

global choice (“which mode?”) is made **early**; fine position is refined **late** — an observation, not a law

Relation to denoising autoencoders

D DERIVATION

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the extra ingredients: a **sequence** of levels, **time conditioning**, and **sampling from noise**

The variational perspective, placed

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connect to the ELBO from L19 — we do **not** re-derive the whole bound here

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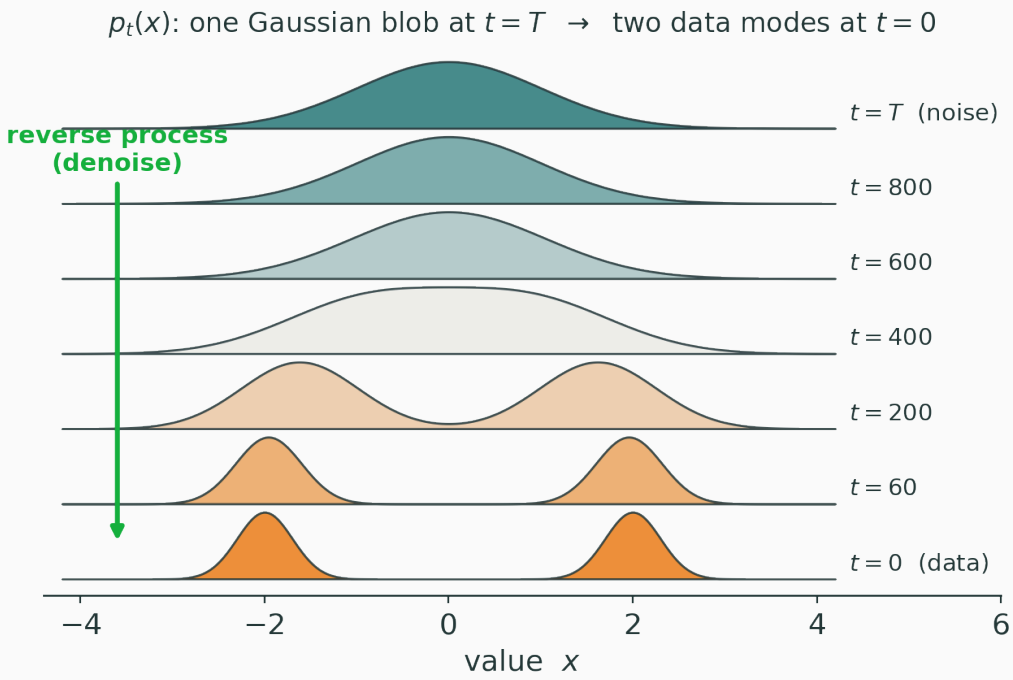

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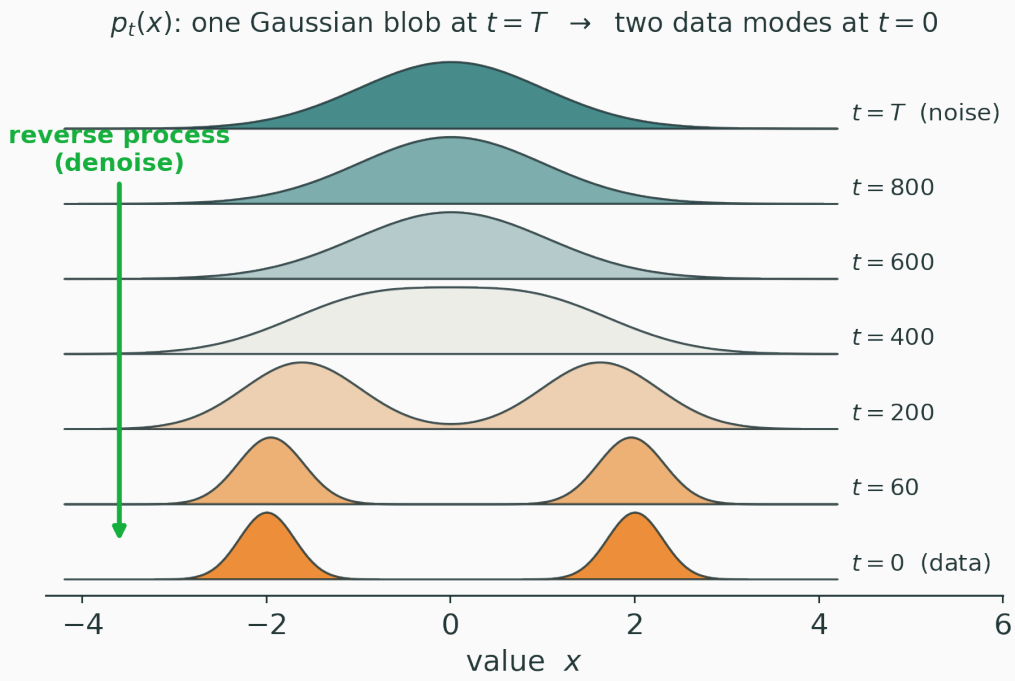

the reverse process rides these directions from one blurry blob back to the data modes

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INTERACTIVE

↗ nipunbatra.github.io/interactive-articles/classifier-guidance

A conditioning widget: watch the reverse trajectory bend toward a chosen class.

Classifier guidance, previewed

D DERIVATION

An external classifier can push the trajectory toward a target class:

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add this to the score to **steer** sampling — L22 teaches the practical **classifier-free** version

Architectural preview: the denoiser

V VISUAL

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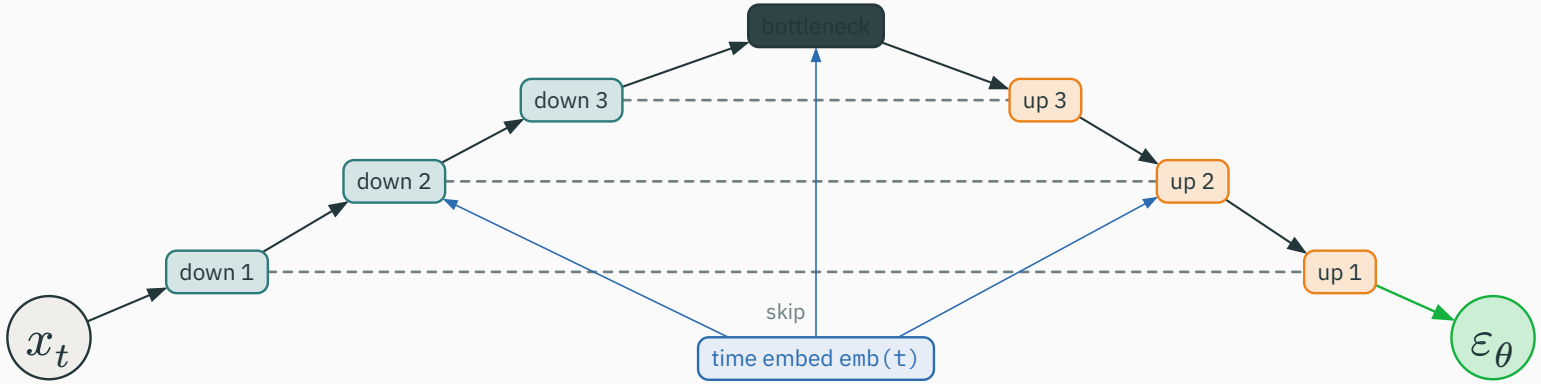

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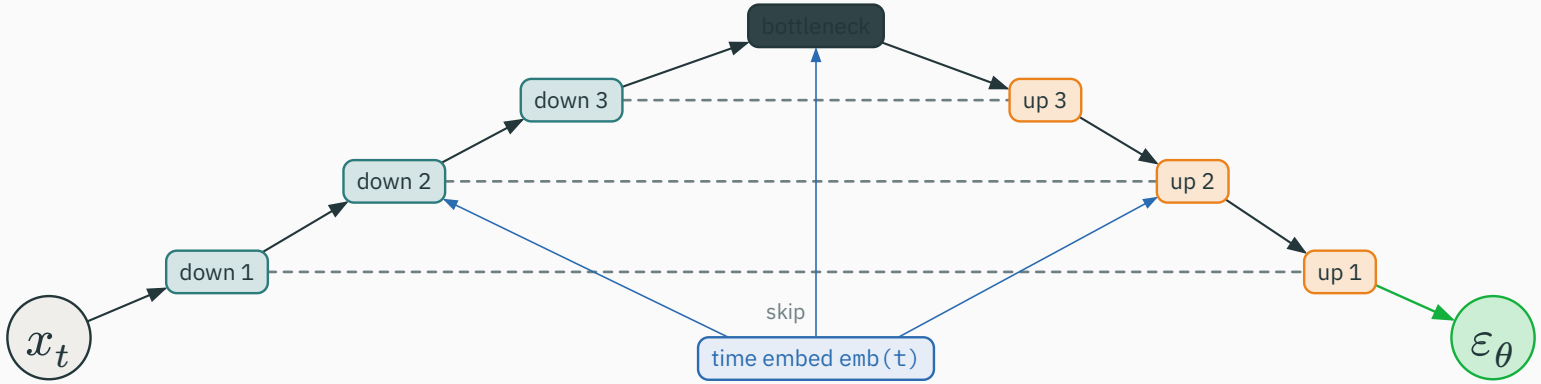

a **U-Net** (or diffusion Transformer): multi-scale, skip connections, time embedding in every block

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Unlike a GAN, **no learned opponent** shifts the target between batches — there is no minimax game to diverge.

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Every example has a **fixed, known** target:

$$\text{target} = \varepsilon \qquad \text{(the noise we drew — it never moves)}$$

Unlike a GAN, **no learned opponent** shifts the target between batches — there is no minimax game to diverge.

optimization is not **trivial**, but the central instability of adversarial training is **gone**

Why diffusion sampling is expensive

V VISUAL

Model family	**Typical generation structure**
VAE	one decode
GAN	one generator pass
diffusion	**repeated** denoiser calls (T of them)

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the model trades **inference work** for a **tractable, stable** training signal

Common misconceptions

Q QUESTION

Misconception	**Correction**
diffusion memorizes a reverse “noise table”	a network **generalizes** denoising across inputs and conditions
the forward process is learned	in standard DDPMs it is **chosen and fixed**
the network only predicts the clean image	noise, clean image, or velocity can be parameterized
more steps always mean a better image	schedules and samplers set a quality / latency **trade-off**

Retrieval questions

Q QUESTION

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Retrieval questions

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if all four are quick to answer, the core of the lecture is secure

The β_t schedule is a design choice

D DERIVATION

The schedule sets the **sequence of learning problems**:

The β_t schedule is a design choice

D DERIVATION

The schedule sets the **sequence of learning problems**:

too little noise — x_T stays structured; the prior $\mathcal{N}(0, I)$ is a poor starting point.

too abrupt noise — intermediate denoising tasks become needlessly hard.

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too little noise — x_T stays structured; the prior $\mathcal{N}(0, I)$ is a poor starting point.

too abrupt noise — intermediate denoising tasks become needlessly hard.

smooth schedules (linear, cosine) spread difficulty **evenly** across timesteps

Variance in reverse sampling

D DERIVATION

The learned reverse Gaussian has a mean **and** a variance:

Variance in reverse sampling

D DERIVATION

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- it controls how much randomness each reverse step injects.

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variance is a **modeling knob**, not an arbitrary visual-effect dial

Loss weighting across timesteps

D DERIVATION

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reweighting timesteps trades off **coarse structure** against **fine detail** quality

Data modalities beyond images

D DERIVATION

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Data modalities beyond images

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The same recipe travels — only the denoiser and conditioning change:

- **audio** waveforms or spectrograms; **video** with temporal structure;
- **molecular** coordinates; **trajectories** and actions; continuous **latent** representations.

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D DERIVATION

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for standard continuous-data DDPMs, forward = Gaussian corruption; the **architecture** must respect the data's structure

Why direct pixel diffusion is demanding

D DERIVATION

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this pressure motivates L22′s **latent-space** diffusion and multi-scale architectures

A tiny one-dimensional thought experiment

V VISUAL

Data lives near -2 and $+2$ on a line; at high noise the two modes **blend**:

A tiny one-dimensional thought experiment

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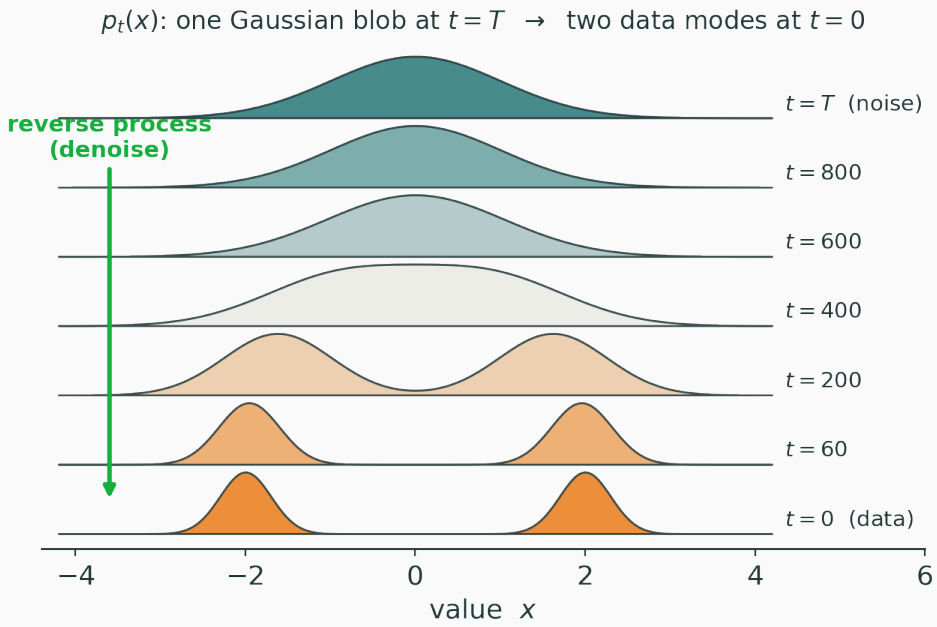

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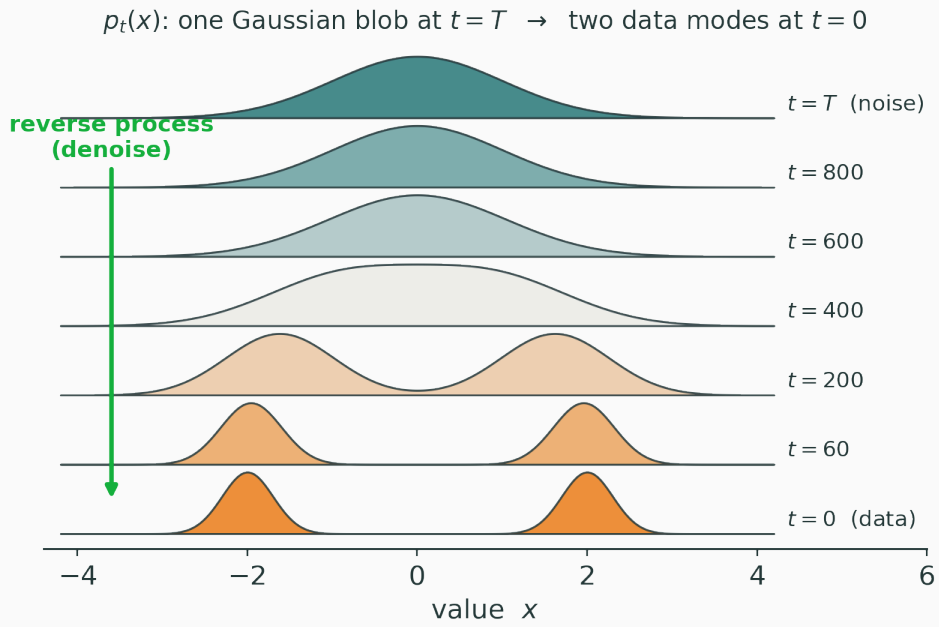

the reverse model must **decide which mode** a noisy point should approach — generation is inherently probabilistic

Denoising is not a nearest-neighbour lookup

D DERIVATION

For a noisy point between modes, the model uses **learned structure**, not a database:

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- the result may resemble **interpolation**, **recombination**, or a genuinely **new** sample;

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D DERIVATION

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- the result may resemble **interpolation**, **recombination**, or a genuinely **new** sample;

Separately: **memorization** remains an empirical risk to **test for** on small or narrow datasets.

A diffusion evaluation lens

Q QUESTION

No single grid or scalar settles quality — evaluate along five axes:

A diffusion evaluation lens

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- **fidelity**; **coverage / diversity**; **conditioning adherence**;
- **sampling cost**; **robustness and harmful failure modes**.

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FID and a caption match tell you **something** — never **everything**

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V VISUAL

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these five coordinates place nearly **every** diffusion system in the course map

Common equations, one page

V VISUAL

Idea	Equation
forward step	$q(x_t \mid x_{t-1}) = \mathcal{N}\left(\sqrt{1-\beta_t}\, x_{t-1}, \beta_t I\right)$
closed form	$x_t = \sqrt{\overline{\alpha}_t}\, x_0 + \sqrt{1-\overline{\alpha}_t}\, \varepsilon$
training loss	$L = \mathbb{E}\left\|\varepsilon - \varepsilon_{\theta(x_t,t)}\right\|_2^2$
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a final reference — **not** another derivation

Retrieval questions, extended

Q QUESTION

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Retrieval questions, extended

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2. How does the closed form turn one image into **many** training examples?
3. Why is the reverse direction **conditional and probabilistic**?
4. What trade-off does **iterative sampling** introduce?

Next lecture

D DERIVATION

noise-prediction objective

$+$ latent space, U-Net / Transformer, and conditioning

$=$ a **practical** diffusion system

Next lecture

D DERIVATION

noise-prediction objective

+ latent space, U-Net / Transformer, and conditioning

= a **practical** diffusion system

L22 builds that system component by component — including **Stable Diffusion**

If you know how to **add** noise, you can train a network to **remove** it.

Next: **Diffusion in practice** → latent diffusion, U-Nets, guidance, and Stable Diffusion.