Generative models for images II

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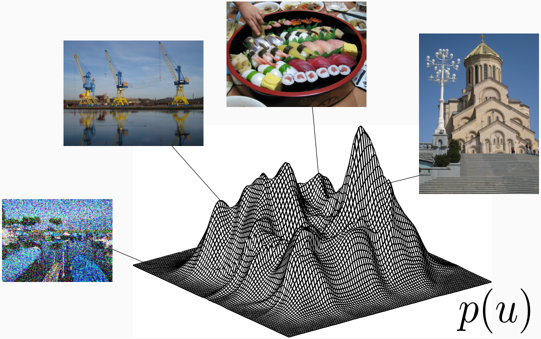
Material for the course is here:
https://www.idpoisson.fr/galerne/caen2024/index.html

Generative models

1. Model and/or learn a distribution $p(u)$ on the space of images.



(source: Charles Deledalle)

The images may represent:

- different instances of the same texture image,
- all images naturally described by a dataset of images,
- any image

2. Generate samples from this distribution.

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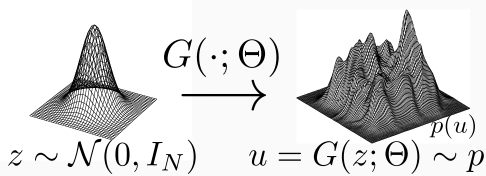

- z is a generic source of randomness, often called the latent variable.
- If $G(\cdot;\Theta)$ is known, then $p = G(\cdot;\Theta)_{\#}\mathcal{N}(0, I_n)$ is the push-forward of the latent distribution.

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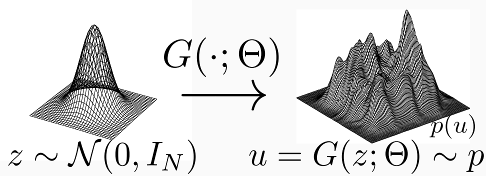

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The generator $G(\cdot;\Theta)$ can be:

- A deterministic function (e.g. convolution operator),
- A neural network with learned parameter,
- An iterative optimization algorithm (gradient descent,...),
- A stochastic sampling algorithm (e.g. MCMC, Langevin diffusion,...).

Basics on diffusion models

Adding noise to images

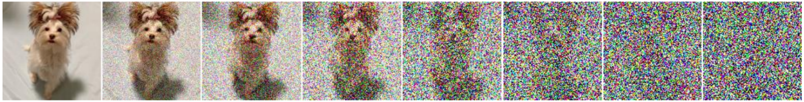
- We are given an input dataset

$$\mathcal{D} = \{\boldsymbol{x}^{(i)},\ i = 1, \dots, N\} \subset \mathbb{R}^d$$

- We assume that these images are independent samples of a common distribution p_0 over $\mathbb{R}^d$.
- Consider the random process that consists of adding noise to images:

$$\boldsymbol{x}_t = \boldsymbol{x}_0 + \boldsymbol{w}_t, \quad t \in [0, T]$$

where $\boldsymbol{x}_0 \sim p_0$ is a sample image and $\boldsymbol{w}_t$ is a Brownian motion (also called Wiener process).



(source: (Song et al., 2021b))

Real-valued: A standard (real-valued) **Brownian motion** (also called **Wiener process** is a stochastic process $(w_t)_{t\geq 0}$ such that

- $w_0 = 0$.
- With probability one, the function $t \mapsto w_t$ is continuous.
- The process $(w_t)_{t\geq 0}$ has stationary independent increments.
- $w_t \sim \mathcal{N}(0, t)$.

Direct consequences:

- For $s < t$, w_s and $w_t - w_s$ are independent and $w_{t-s} \sim \mathcal{N}(0, t - s)$.
- Markovian random field.

$\mathbb{R}^d$**-valued:** A standard $\mathbb{R}^d$-valued Brownian motion $(\boldsymbol{w}_t)_{t\geq 0}$ is made of d independent real-valued Brownian motions

$$\boldsymbol{w}_t = (w_{t,1}, \dots, w_{t,d}) \in \mathbb{R}^d.$$

Ito integral on $[0, T]$:

Given a process $(\boldsymbol{x}_t)_{t\in[0,T]}$ adapted to the filtration $\mathcal{F}_t = \sigma(\boldsymbol{w}_s, s \leq t)$, one defines

$$\int_0^t \boldsymbol{x}_s d\boldsymbol{w}_s \quad \text{as the } L^2 \text{ limit of} \quad \sum_{j=0}^{k-1} \boldsymbol{x}_{t_j} \odot (\boldsymbol{w}_{t_{j+1}} - \boldsymbol{w}_{t_j})$$

when the minimal step of the partition $0 \leq t_0 \leq \cdots \leq t_k \leq T$ tends to 0.

- In particular, for a deterministic function $s \mapsto g(s)$, $\int_0^t g(s) d\boldsymbol{w}_s$ is a normal variable with mean 0 and variance $\sigma^2 = \int_0^t g^2(s) ds$.

Adding noise to images

- Adding noise to images: $\boldsymbol{x}_t = \boldsymbol{x}_0 + \boldsymbol{w}_t, \quad t \in [0, T]$.
- This corresponds to the stochastic differential equation (SDE):

$$d\boldsymbol{x}_t = d\boldsymbol{w}_t \quad \text{with initial condition } \boldsymbol{x}_0 \sim p_0.$$

- We denote by p_t the distribution of $\boldsymbol{x}_t$ at time $t \in [0, T]$. What is p_t?

$$p_t = p_0 * \mathcal{N}(\mathbf{0}, tI_d)$$

- This corresponds to applying the heat equation starting from p_0:

$$\partial_t p_t(\boldsymbol{x}) = \frac{1}{2}\Delta_{\boldsymbol{x}} p_t(\boldsymbol{x}) \quad \text{with } p_{t=0} = p_0.$$

  This PDE is called the **Fokker-Planck equation** associated with the SDE.
- This is an example of diffusion equation.

Diffusion SDE and Fokker-Planck equation

- More generally we will consider diffusion SDE of the form (Song et al., 2021b):

$$d\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_t, t)dt + g(t)d\boldsymbol{w}_t$$

  where

  - $\boldsymbol{f} : \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$ is called the **drift**: External deterministic force that drives $\boldsymbol{x}_t$ in the direction $\boldsymbol{f}(\boldsymbol{x}_t, t)$,
  - $g : [0, T] \to [0, +\infty)$ is the **diffusion coefficient**.

- The corresponding Fokker-Planck equation is

$$\partial_t p_t(\boldsymbol{x}) = -\operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, t) p_t(\boldsymbol{x})\right) + \frac{1}{2} g(t)^2 \Delta_{\boldsymbol{x}} p_t(\boldsymbol{x})$$

  that is,

$$\partial_t p_t(\boldsymbol{x}) = -\sum_{k=1}^{d} \partial_{\boldsymbol{x}_k} \left[\boldsymbol{f}_k(\boldsymbol{x}, t) p_t(\boldsymbol{x})\right] + \frac{1}{2} g(t)^2 \sum_{k=1}^{d} \partial^2_{\boldsymbol{x}_k} p_t(\boldsymbol{x}).$$

Diffusion SDE: Two examples

$$d\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_t, t)dt + g(t)d\boldsymbol{w}_t$$

Example 1: Variance exploding diffusion (VE-SDE)

SDE:	$d\boldsymbol{x}_t = d\boldsymbol{w}_t$
Solution:	$\boldsymbol{x}_t = \boldsymbol{x}_0 + \boldsymbol{w}_t$
Variance:	$\mathrm{Var}(\boldsymbol{x}_t) = \mathrm{Var}(\boldsymbol{x}_0) + t$

Example 2: Variance preserving diffusion (VP-SDE)

SDE:	$d\boldsymbol{x}_t = -\beta_t \boldsymbol{x}_t dt + \sqrt{2\beta_t} d\boldsymbol{w}_t$
Solution:	$\boldsymbol{x}_t = e^{-B_t}\boldsymbol{x}_0 + \int_0^t e^{B_s - B_t}\sqrt{2\beta_s} d\boldsymbol{w}_s$ with $B_t = \int_0^t \beta_s ds$
Variance:	$\mathrm{Var}(\boldsymbol{x}_t) = e^{-2B_t}\mathrm{Var}(\boldsymbol{x}_0) + 1 - e^{-2B_t}$ $= 1$ if $\mathrm{Var}(\boldsymbol{x}_0) = 1.$

Both variants have the form $\boldsymbol{x}_t = a_t \boldsymbol{x}_0 + b_t \boldsymbol{Z}_t$: $\boldsymbol{x}_t$ is a rescaled noisy version of $\boldsymbol{x}_0$ and the noise is more and more predominant as time grows.

Numerical scheme for diffusion SDE

$$d\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_t, t)dt + g(t)d\boldsymbol{w}_t$$

In general we do not have a close form formula for $\boldsymbol{x}_t$.

Diffusion SDEs can be approximately simulated using numerical schemes such as the **Euler-Maruyama sheme**:

- Using the time step $h = T/N$ with $N+1$ times $t_n = nh$, $n \in \{0, \dots N\}$, define $\boldsymbol{X}_0 = \boldsymbol{x}_0$ and

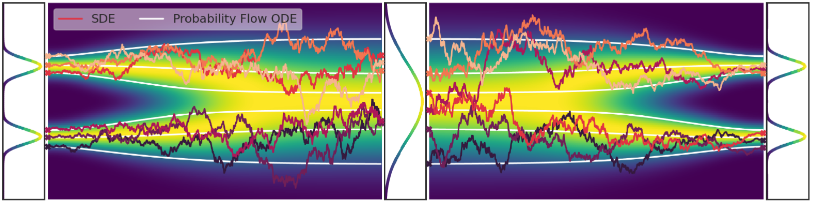
$$\boldsymbol{X}_{n+1} = \boldsymbol{X}_n + \boldsymbol{f}(\boldsymbol{X}_n, t_n)h + g(t_n)\left(\boldsymbol{w}_{t_{n+1}} - \boldsymbol{w}_{t_n}\right), \quad n = 1, \dots, N-1.$$

- Remark that $\boldsymbol{w}_{t_{n+1}} - \boldsymbol{w}_{t_n} \sim \mathcal{N}(\boldsymbol{0}, hI_d)$ and is independent of $\boldsymbol{X}_n$:

$$\boldsymbol{X}_{n+1} = \boldsymbol{X}_n + \boldsymbol{f}(\boldsymbol{X}_n, t_n)h + g(t_n)\sqrt{h}\boldsymbol{Z}_n, \quad \text{with } \boldsymbol{Z}_n \sim \mathcal{N}(\boldsymbol{0}, I_d), \quad n = 1, \dots, N-1.$$

Reversed diffusion

- For diffusion SDEs, as t grows p_t is closer and closer to a normal distribution.
- We will consider that at the final time $t = T$ large enough so that p_T can be considered to be a normal distribution.
- For generative modeling, we want to reverse the process:
  - Start by generating $\boldsymbol{x}_T \sim p_T \approx \mathcal{N}(\mathbf{0}, \sigma_T^2 I_d)$.
  - Simulate $(\boldsymbol{x}_{T-t})_{t\in[0,T]}$ such that $\boldsymbol{x}_{T-t} \sim p_{T-t}$.



(source: (Song and Ermon, 2020))

Reversed diffusion

Reversed diffusion: What is the SDE satisfied by $\boldsymbol{x}_{T-t}$?

$$d\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_t, t)dt + g(t)d\boldsymbol{w}_t$$

has the associated Fokker-Planck equation

$$\partial_t p_t(\boldsymbol{x}) = -\operatorname{div}_{\boldsymbol{x}}\left(\boldsymbol{f}(\boldsymbol{x}, t)p_t(\boldsymbol{x})\right) + \frac{1}{2}g(t)^2\Delta_{\boldsymbol{x}} p_t(\boldsymbol{x}).$$

Let us derive the Fokker-Planck equation for $q_t = p_{T-t}$ the distribution function of $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$.

$$\begin{aligned}
&\partial_t q_t(\boldsymbol{x}) = -\partial_t p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}}\left(\boldsymbol{f}(\boldsymbol{x}, T-t)p_{T-t}(\boldsymbol{x})\right) - \frac{1}{2}g(T-t)^2\Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}}\left(\boldsymbol{f}(\boldsymbol{x}, T-t)q_t(\boldsymbol{x})\right) - \frac{1}{2}g(T-t)^2\Delta_{\boldsymbol{x}} q_t(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}}\left(\boldsymbol{f}(\boldsymbol{x}, T-t)q_t(\boldsymbol{x})\right) + \left(-1 + \frac{1}{2}\right)g(T-t)^2\Delta_{\boldsymbol{x}} q_t(\boldsymbol{x})
\end{aligned}$$

Reversed diffusion

$$\begin{aligned}
&\partial_t q_t(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) q_t(\boldsymbol{x})\right) + \left(-1 + \frac{1}{2}\right) g(T-t)^2 \Delta_{\boldsymbol{x}} q_t(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) q_t(\boldsymbol{x}) - g(T-t)^2 \nabla_{\boldsymbol{x}} q_t(\boldsymbol{x})\right) + \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} q_t(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\left[\boldsymbol{f}(\boldsymbol{x}, T-t) - g(T-t)^2 \frac{\nabla_{\boldsymbol{x}} q_t(\boldsymbol{x})}{q_t(\boldsymbol{x})}\right] q_t(\boldsymbol{x})\right) + \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} q_t(\boldsymbol{x}) \\
&= -\operatorname{div}_{\boldsymbol{x}} \left(\left[-\boldsymbol{f}(\boldsymbol{x}, T-t) + g(T-t)^2 \nabla_{\boldsymbol{x}} \log q_t(\boldsymbol{x})\right] q_t(\boldsymbol{x})\right) + \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} q_t(\boldsymbol{x})
\end{aligned}$$

This is the Fokker-Planck equation associated with the diffusion SDE:

$$d\boldsymbol{y}_t = \left[-\boldsymbol{f}(\boldsymbol{y}_t, T-t) + g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t)\right] dt + g(T-t) d\boldsymbol{w}_t.$$

Reversed diffusion

Forward diffusion:

$$d\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_t, t)dt + g(t)d\boldsymbol{w}_t$$

Backward diffusion: $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$

$$d\boldsymbol{y}_t = \left[-\boldsymbol{f}(\boldsymbol{y}_t, T-t) + g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t)\right] dt + g(T-t)d\boldsymbol{w}_t.$$

- Same diffusion coefficient.
- Opposite drift term with additional distribution correction:

$$g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t)$$

  drives the diffusion in regions with high p_{T-t} probability.
- $\boldsymbol{x} \mapsto \nabla_{\boldsymbol{x}} \log p_t(\boldsymbol{x})$ is called the (Stein) **score** of the distribution.
- Rigorous results from SDE litterature ((Anderson, 1982) (Haussmann and Pardoux, 1986)) (measurability issues, the filtration is also reversed...).

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Forward diffusion:

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- Rigorous results from SDE litterature ((Anderson, 1982) (Haussmann and Pardoux, 1986)) (measurability issues, the filtration is also reversed...).
- Can we simulate this backward diffusion using Euler-Maruyama ?

$$\boldsymbol{X}_{n+1} = \boldsymbol{X}_n + \boldsymbol{f}(\boldsymbol{X}_n, t_n)h + g(t)\sqrt{h}\boldsymbol{Z}_n, \quad \text{with } Z_n \sim \mathcal{N}(\boldsymbol{0}, I_d), \quad n = 1, \dots, N-1.$$

Learning the score function: Denoising score matching

- **Goal:** Estimate the score $\boldsymbol{x} \mapsto \nabla_{\boldsymbol{x}} \log p_t(\boldsymbol{x})$ using only available samples $(\boldsymbol{x}_0, \boldsymbol{x}_t)$.
- For the models of interests, $\boldsymbol{x}_t = a_t \boldsymbol{x}_0 + b_t \boldsymbol{Z}_t$ is a rescaled noisy version of $\boldsymbol{x}_0$ (both a_t and b_t have known analytical expressions).
- Explicit conditional distribution: $p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0) = \mathcal{N}(a_t\boldsymbol{x}_0, b_t^2 I_d)$.

$$
\begin{aligned}
p_t(\boldsymbol{x}_t) &= \int_{\mathbb{R}^d} p_{0,t}(\boldsymbol{x}_0, \boldsymbol{x}_t) d\boldsymbol{x}_0 = \int_{\mathbb{R}^d} p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0) p_0(\boldsymbol{x}_0) d\boldsymbol{x}_0 \\
\nabla_{\boldsymbol{x}_t} p_t(\boldsymbol{x}_t) &= \int_{\mathbb{R}^d} \nabla_{\boldsymbol{x}_t} p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0) p_0(\boldsymbol{x}_0) d\boldsymbol{x}_0 \\
\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t) = \frac{\nabla_{\boldsymbol{x}_t} p_t(\boldsymbol{x}_t)}{p_t(\boldsymbol{x}_t)} &= \int_{\mathbb{R}^d} \nabla_{\boldsymbol{x}_t} p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0) \frac{p_0(\boldsymbol{x}_0)}{p_t(\boldsymbol{x}_t)} d\boldsymbol{x}_0 \\
&= \int_{\mathbb{R}^d} \left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\right] p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0) \frac{p_0(\boldsymbol{x}_0)}{p_t(\boldsymbol{x}_t)} d\boldsymbol{x}_0 \\
&= \int_{\mathbb{R}^d} \left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\right] p_{0|t}(\boldsymbol{x}_0|\boldsymbol{x}_t) d\boldsymbol{x}_0
\end{aligned}
$$

Conclusion:

$$
\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t) = \mathbb{E}_{\boldsymbol{x}_0 \sim p_{0|t}(\boldsymbol{x}_0|\boldsymbol{x}_t)} \left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\right] = \mathbb{E}\left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0) | \boldsymbol{x}_t\right]
$$

Learning the score function: Denoising score matching

$$\boxed{\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t) = \mathbb{E}_{\boldsymbol{x}_0 \sim p_{0|t}(\boldsymbol{x}_0|\boldsymbol{x}_t)} \left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\right] = \mathbb{E}\left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)|\boldsymbol{x}_t\right]}$$

- $\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)$ is explicit (forward transition): For $\boldsymbol{x}_t|\boldsymbol{x}_0 \sim \mathcal{N}(\alpha_t \boldsymbol{x}_0, \beta_t^2 I_d)$,

$$\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0) = \nabla_{\boldsymbol{x}_t} \left[-\frac{1}{2\beta_t^2} \left\|\boldsymbol{x}_t - \alpha_t \boldsymbol{x}_0\right\|^2 + C\right] = -\frac{1}{\beta_t^2} \left(\boldsymbol{x}_t - \alpha_t \boldsymbol{x}_0\right) = -\frac{1}{\beta_t} \boldsymbol{Z}_t$$

- But the distribution $p_{0|t}(\boldsymbol{x}_0|\boldsymbol{x}_t)$ is not explicit (backward conditional)!

$$\mathbb{E}\left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)|\boldsymbol{x}_t\right] = -\frac{1}{\beta_t^2} \left(\boldsymbol{x}_t - \alpha_t \mathbb{E}[\boldsymbol{x}_0|\boldsymbol{x}_t]\right)$$

- $\mathbb{E}[\boldsymbol{x}_0|\boldsymbol{x}_t]$ is the best estimate of the initial noise-free $\boldsymbol{x}_0$ given its noisy version $\boldsymbol{x}_t$.

Learning the score function: Denoising score matching

$$\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t) = \mathbb{E}_{\boldsymbol{x}_0 \sim p_{0|t}(\boldsymbol{x}_0|\boldsymbol{x}_t)} \left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\right] = \mathbb{E}\left[\nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)|\boldsymbol{x}_t\right]$$

We use the following properties of the **conditional expectation**.

- $Y = \mathbb{E}[X|\mathcal{F}]$ if and only if $Y = \operatorname{argmin}\{\mathbb{E}\|X - Z\|^2,\ Z \in \mathrm{L}^2(\mathcal{F})\}$.
- $Y \in \sigma(X)$ iif there exists $f:\ \mathbb{R}^d \to \mathbb{R}^d$ (measurable) with $Y = f(X)$.
- $Y = \mathbb{E}[X|U]$ if $Y = f(U)$ with $f = \operatorname{argmin}\{\mathbb{E}\|X - f(U)\|^2,\ f \in \mathrm{L}^2(U)\}$.

Hence the function $\boldsymbol{x}_t \mapsto \nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t)$ is the solution

$$\nabla_{\boldsymbol{x}_t} \log p_t = \operatorname{argmin}\{\mathbb{E}_{p_{0,t}} \|f(\boldsymbol{x}_t) - \nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2,\ f \in \mathrm{L}^2(p_t)\}$$

- We obtain a **loss function** to learn the function f using Monte Carlo approximation with samples $(\boldsymbol{x}_0, \boldsymbol{x}_t)$ for the expectation.

Learning the score function: Denoising score matching

$$\nabla_{\boldsymbol{x}_t} \log p_t = \operatorname{argmin}\{\mathbb{E}_{p_{0,t}} \|f(\boldsymbol{x}_t) - \nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2, \ f \in \mathrm{L}^2(p_t)\}$$

- $f : \mathbb{R}^d \to \mathbb{R}^d$ will be approximated with a neural network such as a (complex) U-net (Ho et al., 2020).
- But we need to have an approximation of $\nabla_{\boldsymbol{x}_t} \log p_t$ for all time t (at least for the times t_n in our Euler-Maruyama scheme).
- In practice we share the same network architecture for all time t: one learns a network $\boldsymbol{s}_\theta(\boldsymbol{x}, t)$ such that

$$\boldsymbol{s}_\theta(\boldsymbol{x}, t) \approx \nabla_{\boldsymbol{x}} \log p_t(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d, \ t \in [0, T].$$

Final loss for denoising score matching: (Song et al., 2021b)

$$\theta^* = \operatorname{argmin} \mathbb{E}_t \left(\lambda_t \mathbb{E}_{(\boldsymbol{x}_0, \boldsymbol{x}_t)} \|\boldsymbol{s}_\theta(\boldsymbol{x}_t, t) - \nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2 \right)$$

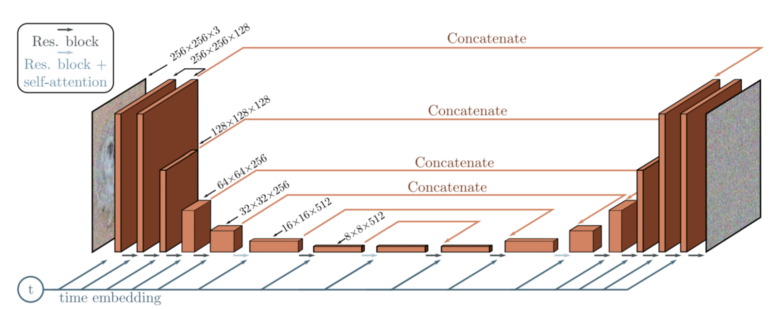
where t is chosen uniformly in $[0, T]$ and $t \mapsto \lambda_t$ is a weighting term to balance the importance of each t.

Practical aspects of diffusion models: Training and sampling

Score architecture

$$\theta^* = \operatorname{argmin} \mathbb{E}_t \left(\lambda_t \mathbb{E}_{(\boldsymbol{x}_0, \boldsymbol{x}_t)} \| s_\theta(\boldsymbol{x}_t, t) - \nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t | \boldsymbol{x}_0) \|^2 \right)$$

- $s_\theta : \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$ is a (complex) U-net (Ronneberger et al., 2015), eg in (Ho et al., 2020) "All models have two convolutional residual blocks per resolution level and self-attention blocks at the 16×16 resolution between the convolutional blocks".
- Diffusion time t is specified by adding the Transformer sinusoidal position embedding into each residual block (Vaswani et al., 2017).



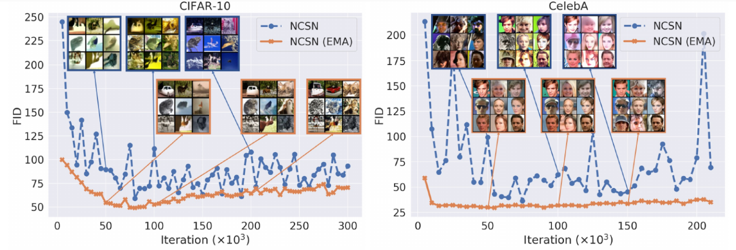
(source: learnopencv.com)

Exponential Moving Average

- Several choices for $t \mapsto \lambda_t$, linked to ELBO and data augmentation (Kingma and Gao, 2023).
- Training using Adam algorithm (Kingma and Ba, 2015), but still **unstable**.
- To regularize: **E**xponential **M**oving **A**verage (EMA) of weights.

$$\bar{\theta}_{n+1} = (1 - m)\bar{\theta}_n + m\theta_n.$$

- Typically $m = 10^{-4}$ (more than 10^4 iterations are averaged).
- The final averaged parameters $\bar{\theta}_K$ are used at **sampling**.



Training instabilities (source: (Song and Ermon, 2020))

Sampling strategy

- The score function of a distribution is generally used for Langevin sampling (ULA or MALA):

$$\boldsymbol{X}_{n+1} = \boldsymbol{X}_n + \gamma \nabla_{\boldsymbol{x}} \log p(\boldsymbol{X}_n) + \sqrt{2\gamma}\boldsymbol{Z}_n$$

- (Song et al., 2021b) propose to add one step of Langevin diffusion (same $t = t_n$) after each step Euler-Maruyama step (t_n to t_{n+1}).
- This means that we jump from one trajectory to the other, but we correct some defaults from the Euler scheme.
- This is called a Predictor-Corrector sampler.

Algorithm 2 PC sampling (VE SDE)

$\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \sigma_{\max}^2 \mathbf{I})$
for $i = N-1$ **to** 0 **do**
  $\mathbf{x}'_i \leftarrow \mathbf{x}_{i+1} + (\sigma_{i+1}^2 - \sigma_i^2)\mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_{i+1}, \sigma_{i+1})$
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  $\mathbf{x}_i \leftarrow \mathbf{x}'_i + \sqrt{\sigma_{i+1}^2 - \sigma_i^2}\,\mathbf{z}$
  for $j = 1$ **to** M **do**
    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
    $\mathbf{x}_i \leftarrow \mathbf{x}_i + \epsilon_i \mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_i, \sigma_i) + \sqrt{2\epsilon_i}\,\mathbf{z}$
return $\mathbf{x}_0$

Algorithm 3 PC sampling (VP SDE)

$\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $i = N-1$ **to** 0 **do**
  $\mathbf{x}'_i \leftarrow (2 - \sqrt{1 - \beta_{i+1}})\mathbf{x}_{i+1} + \beta_{i+1}\mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_{i+1}, i+1)$
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  $\mathbf{x}_i \leftarrow \mathbf{x}'_i + \sqrt{\beta_{i+1}}\,\mathbf{z}$ — Predictor
  for $j = 1$ **to** M **do** — Corrector
    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
    $\mathbf{x}_i \leftarrow \mathbf{x}_i + \epsilon_i \mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_i, i) + \sqrt{2\epsilon_i}\,\mathbf{z}$
return $\mathbf{x}_0$

(source: (Song et al., 2021b))

Results

- (Song et al., 2021b) achieved SOTA in terms of FID for CIFAR-10 unconditional sampling.
- Very good results for 1024×1024 portrait images.
- See also "Diffusion Models Beat GANs on Image Synthesis" (Dhariwal and Nichol, 2021) (self-explanatory title).

(source: FFHQ 1024×1024 samples (Song et al., 2021b))

Many approximations

Many approximations in the full generative pipelines:

- The final distribution p_T is not exactly a normal distribution.
- The learnt Unet model s_θ is far from being the exact score function: Sample-based, limitations from the architecture...
- Discrete sampling scheme (Euler-Maruyama, Predictor-Corrector,...).
- Score function may behave badly near $t = 0$ (irregular density in case of manifold hypothesis).

But we do have theoretical guarantees if all is well controled!

Theorem (Convergence guarantees (De Bortoli, 2022))
Let p_0 be the data distribution having a compact manifold support and let q_T be the generator distribution from the reversed diffusion. Under suitable hypotheses, the 1-Wasserstein distance $W_1(p_0, q_T)$ can be explicitly bounded and tends to zero when all the parameters are refined (more Euler steps, better score learning, etc.).

The deterministic approach: Probability flow ODE

Sampling via an ODE

We derived the Fokker-Planck equation for $q_t = p_{T-t}$ of reversed diffusion $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$.

$$\begin{aligned}
&\partial_t q_t(\boldsymbol{x}) = -\partial_t p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x})\right) - \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x})\right) + \left(-1 + \frac{1}{2}\right) g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x}) \\
&= -\operatorname{div}_{\boldsymbol{x}} \left(\left[-\boldsymbol{f}(\boldsymbol{x}, T-t) + g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{x})\right] p_{T-t}(\boldsymbol{x})\right) + \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x})
\end{aligned}$$

This is the Fokker-Planck equation associated with the diffusion SDE:

$$d\boldsymbol{y}_t = \left[-\boldsymbol{f}(\boldsymbol{y}_t, T-t) + g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t)\right] dt + g(T-t) d\boldsymbol{w}_t.$$

Sampling via an ODE

We derived the Fokker-Planck equation for $q_t = p_{T-t}$ of reversed diffusion $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$.

$$\begin{aligned}
&\partial_t q_t(\boldsymbol{x}) = -\partial_t p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x})\right) - \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x})\right) + \left(-1 + \frac{1}{2}\right) g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x})
\end{aligned}$$

Sampling via an ODE

We derived the Fokker-Planck equation for $q_t = p_{T-t}$ of reversed diffusion $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$.

$$\begin{aligned}
&\partial_t q_t(\boldsymbol{x}) = -\partial_t p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}}\left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x})\right) - \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}}\left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x})\right) + \left(-\frac{1}{2} + 0\right) g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x})
\end{aligned}$$

Sampling via an ODE

We derived the Fokker-Planck equation for $q_t = p_{T-t}$ of reversed diffusion $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$.

$$\begin{aligned}
\partial_t q_t(\boldsymbol{x}) &= -\partial_t p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x}) \right) - \frac{1}{2} g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x}) \\
&= \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{f}(\boldsymbol{x}, T-t) p_{T-t}(\boldsymbol{x}) \right) + \left(-\frac{1}{2} + 0 \right) g(T-t)^2 \Delta_{\boldsymbol{x}} p_{T-t}(\boldsymbol{x}) \\
&= -\operatorname{div}_{\boldsymbol{x}} \left(\left[-\boldsymbol{f}(\boldsymbol{x}, T-t) + \frac{1}{2} g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{x}) \right] p_{T-t}(\boldsymbol{x}) \right)
\end{aligned}$$

This is the Fokker-Planck equation associated with the diffusion SDE:

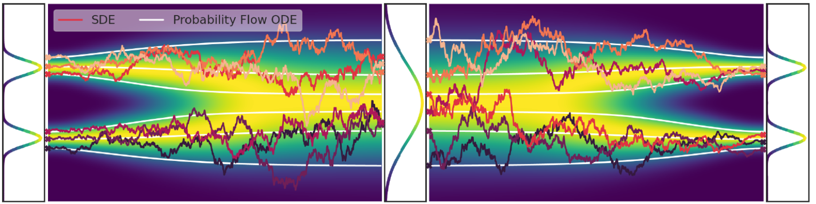
$$d\boldsymbol{y}_t = \left[-\boldsymbol{f}(\boldsymbol{y}_t, T-t) + \frac{1}{2} g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t) \right] dt.$$

which is an **Ordinary Differential Equation (ODE)** (no stochastic term) !

Reverse diffusion via an ODE

$$dy_t = \left[-f(y_t, T-t) + \frac{1}{2}g(T-t)^2\nabla_x \log p_{T-t}(y_t)\right] dt.$$

This ODE is called a **probability flow ODE**.



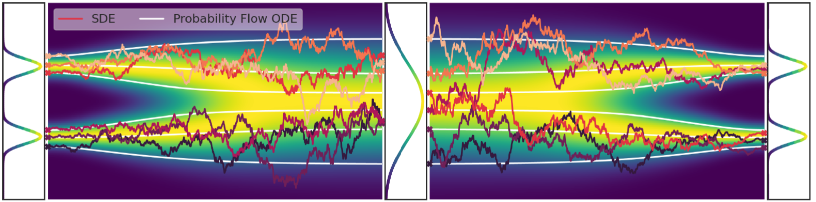
(source: (Song and Ermon, 2020))

- Like with normalizing flows, we get a deterministic mapping between initial noise and generated images.
- We do not simulate the (chaotic) path of the stochastic diffusion **but we still have the same marginal distribution** p_t.
- We can use **any ODE solver**, with higher order than Euler scheme.

Reverse diffusion via an ODE

$$dy_t = \left[-f(y_t, T-t) + \frac{1}{2} g(T-t)^2 \nabla_x \log p_{T-t}(y_t) \right] dt.$$

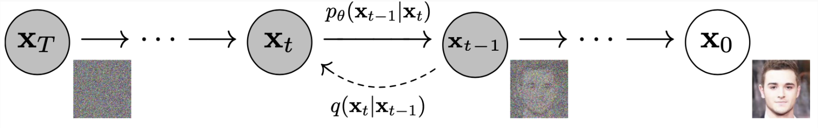
This ODE is called a **probability flow ODE**.



(source: (Song and Ermon, 2020))

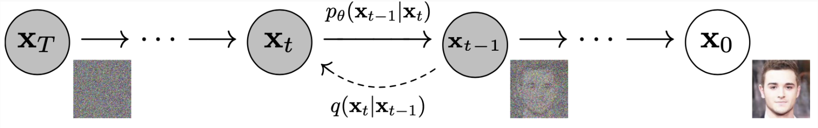
- From (Karras et al., 2022) "Through extensive tests, we have found Heun's 2nd order method (a.k.a. improved Euler, trapezoidal rule) [...] to provide an excellent tradeoff between truncation error and NFE."
- Requires much less NFE than stochastic samplers (eg around 50 steps instead of 1000), see also Denoising Diffusion Implicit Models (DDIM) (Song et al., 2021a) for a deterministic approach.

The discrete approach for diffusion models:
Denoising Diffusion Probabilistic Models



(source: (Ho et al., 2020))

Denoising Diffusion Probabilistic Models (**DDPM** (Ho et al., 2020)) is a discrete model with a fixed number of $T = 10^3$ steps that performs discrete diffusion.



(source: (Ho et al., 2020))

Denoising Diffusion Probabilistic Models (**DDPM** (Ho et al., 2020)) is a discrete model with a fixed number of $T = 10^3$ steps that performs discrete diffusion.

WARNING: Slight change of notation

Forward model: Discrete variance preserving diffusion

- Distribution of samples: $q(\boldsymbol{x}_0)$.
- Conditional Gaussian noise: $q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}\boldsymbol{x}_{t-1}, \beta_t \boldsymbol{I}_d)$

$$\boldsymbol{x}_t = \sqrt{1-\beta_t}\boldsymbol{x}_{t-1} + \sqrt{\beta_t}\boldsymbol{z}_t$$

  where the variance schedule $(\beta_t)_{1 \leq t \leq T}$ is fixed.
- One step noising $q(\boldsymbol{x}_t|\boldsymbol{x}_0)$: With $\alpha_t = 1 - \beta_t$ and $\bar{\alpha} = \mathrm{cumprod}(\alpha)$

$$\boldsymbol{x}_t = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{z} \quad \text{where} \quad \boldsymbol{z} \text{ is standard.}$$

Denoising Diffusion Probabilistic Models

- We consider the diffusion as a fixed stochastic encoder
- We want to learn a **stochastic decoder** p_θ:

$$p_\theta(\boldsymbol{x}_{0:T}) = \underbrace{p(\boldsymbol{x}_T)}_{\text{fixed latent prior}} \prod_{t=1}^{T} \underbrace{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}_{\text{learnable backward transitions}} .$$

$$\text{with} \quad p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) = \mathcal{N}(\mu_\theta(\boldsymbol{x}_t, t), \beta_t \boldsymbol{I}_d)$$

$$\text{Compare with:} \quad q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}\boldsymbol{x}_{t-1}, \beta_t \boldsymbol{I}_d)$$

- Recall same diffusion coefficient, new backward drift to be learnt,...
- Oversimplified version compare to (Ho et al., 2020), there are ways to also learn the variance for each pixel, see (Nichol and Dhariwal, 2021).
- Then we look for training the decoder by maximizing an **ELBO**.

DDPM: Training loss

$$\mathbb{E}(-\log p_\theta(\boldsymbol{x}_0)) \leq \mathbb{E}_q \left[-\log \left[\frac{p_\theta(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right]\right] := L$$

We have

$$L = \mathbb{E}_q \left[-\log p(\boldsymbol{x}_T) - \sum_{t=1}^{T} \log \frac{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right]$$

DDPM: Training loss

$$\mathbb{E}(-\log p_\theta(\boldsymbol{x}_0)) \leq \mathbb{E}_q\left[-\log\left[\frac{p_\theta(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right]\right] := L$$

We have

$$L = \mathbb{E}_q\left[-\log p(\boldsymbol{x}_T) - \sum_{t=1}^{T} \log \frac{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right]$$

$= \dots$ (see (Ho et al., 2020) Appendix A)

DDPM: Training loss

$$\mathbb{E}(-\log p_\theta(\boldsymbol{x}_0)) \leq \mathbb{E}_q\left[-\log\left[\frac{p_\theta(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right]\right] := L$$

We have

$$L = \mathbb{E}_q\left[-\log p(\boldsymbol{x}_T) - \sum_{t=1}^{T} \log \frac{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right]$$

$= \dots$ (see (Ho et al., 2020) Appendix A)

$$= \mathbb{E}_q\Bigg[D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0)\|p(\boldsymbol{x}_T)) + \sum_{t=2}^{T} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\|p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) - \log p_\theta(\boldsymbol{x}_0|\boldsymbol{x}_1)\Bigg]$$

DDPM: Training loss

Computation of $D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\|p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))$

By Bayes rule,

$$q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0) = q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} = q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}$$

Computation shows that this is a normal distribution $\mathcal{N}(\tilde{\mu}(\boldsymbol{x}_t,\boldsymbol{x}_0),\tilde{\beta}_t I_d)$ with

$$\tilde{\mu}(\boldsymbol{x}_t,\boldsymbol{x}_0) = \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\boldsymbol{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\boldsymbol{x}_t \quad \text{and} \quad \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t.$$

Using the expression of the KL-divergence between Gaussian distributions,

$$D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\|p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) = \frac{1}{\beta_t}\left\|\mu_\theta(\boldsymbol{x}_t,t)-\tilde{\mu}(\boldsymbol{x}_t,\boldsymbol{x}_0)\right\|^2 + C$$

$$L_t = \mathbb{E}_q\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\|p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right] = \frac{1}{\beta_t}\mathbb{E}_q\left[\left\|\mu_\theta(\boldsymbol{x}_t,t)-\tilde{\mu}(\boldsymbol{x}_t,\boldsymbol{x}_0)\right\|^2\right] + C$$

DDPM: Noise reparameterization

Rewrite everything **in function of the added standard noise** ε:

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\varepsilon}$$

Then $\mu_\theta(\boldsymbol{x}_t, t)$ must predict

$$\tilde{\mu}(\boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{1}{\sqrt{\alpha_t}}\left(\boldsymbol{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\varepsilon}\right)$$

If we parameterize

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

Then the loss is simply

$$\begin{aligned} L_t &= \frac{\beta_t}{1-\bar{\alpha}_t}\mathbb{E}_q\left[\left\|\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t) - \boldsymbol{\varepsilon}\right\|^2\right] + C \\ &= \frac{\beta_t}{1-\bar{\alpha}_t}\mathbb{E}_{\boldsymbol{x}_0,\boldsymbol{\varepsilon}}\left[\left\|\boldsymbol{\varepsilon}_\theta(\sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\varepsilon}, t) - \boldsymbol{\varepsilon}\right\|^2\right] + C \end{aligned}$$

That is we must predict the noise ε added to $\boldsymbol{x}_0$ (without knowing $\boldsymbol{x}_0$).

DDPM: Training and sampling

$$L = \mathbb{E}_q\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0)\|p(\boldsymbol{x}_T)) + \sum_{t=2}^{T} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\|p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) - \log p_\theta(\boldsymbol{x}_0|\boldsymbol{x}_1) \right]$$

$$= \sum_{t=2}^{T} L_t + L_1 + C$$

- The L_1 term is dealt differently (to account for discretization of $\boldsymbol{x}_0$).
- (Ho et al., 2020) proposes to simplify the loss (no constants):

$$L_{\text{simple}} = \mathbb{E}_{t,\boldsymbol{x}_0,\boldsymbol{\varepsilon}}\left[\left\| \boldsymbol{\varepsilon}_\theta(\sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\varepsilon}, t) - \boldsymbol{\varepsilon} \right\|^2 \right]$$

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1,\dots,T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0},\mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0},\mathbf{I})$
for $t = T,\dots,1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0},\mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here.

(source: (Ho et al., 2020))

DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$

$\boldsymbol{x}_t$ $\quad$ $\hat{\boldsymbol{x}}_0$ $\quad$ $\boldsymbol{x}_0$

$t = 11$

DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

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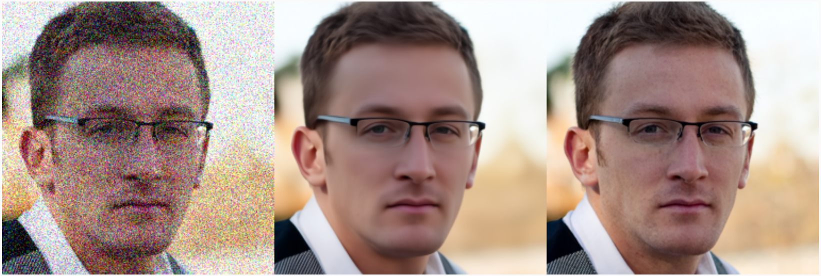


$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_0$

$t = 100$

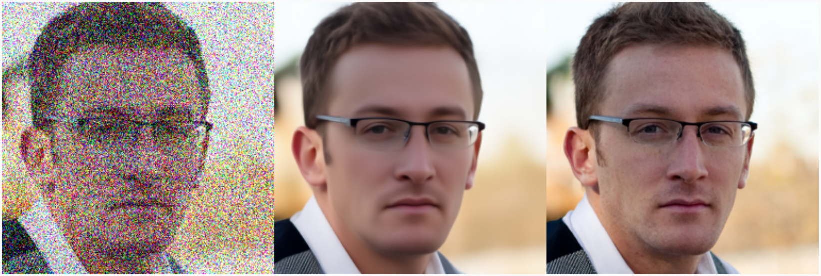
DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$ $\quad$ $\hat{\boldsymbol{x}}_0$ $\quad$ $\boldsymbol{x}_0$

$t = 200$

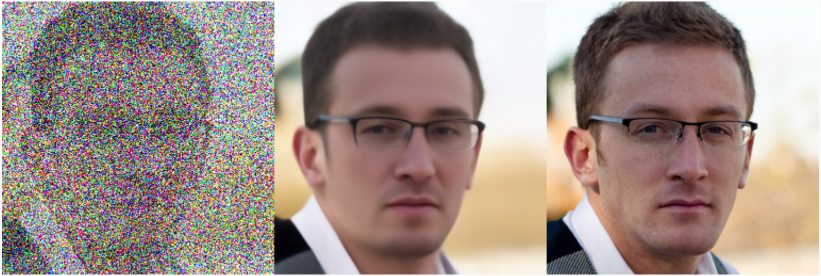
DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$ $\quad$ $\hat{\boldsymbol{x}}_0$ $\quad$ $\boldsymbol{x}_0$

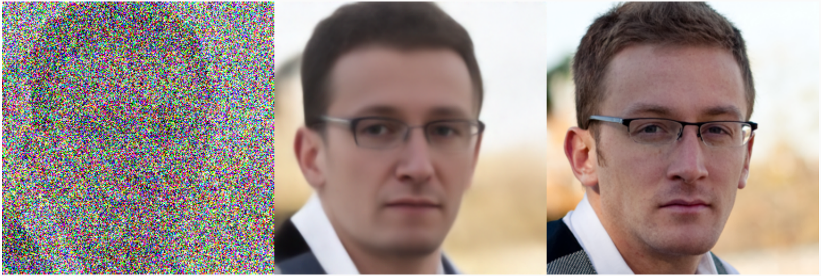
$t = 400$

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$ $\qquad$ $\hat{\boldsymbol{x}}_0$ $\qquad$ $\boldsymbol{x}_0$

$t = 500$

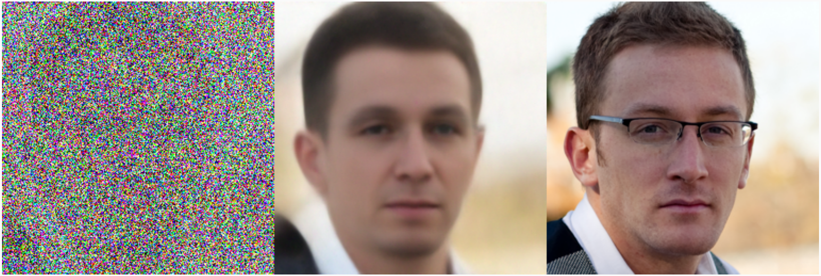
DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$ $\quad$ $\hat{\boldsymbol{x}}_0$ $\quad$ $\boldsymbol{x}_0$

$t = 600$

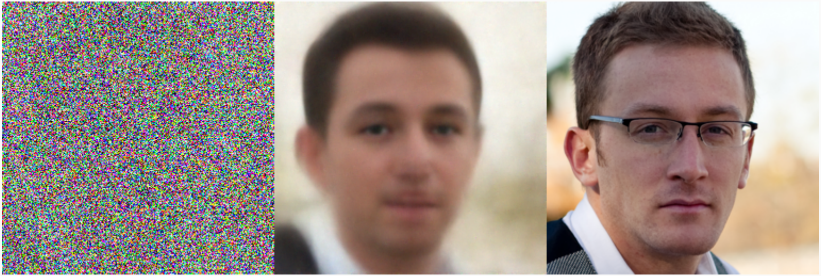
DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_0$

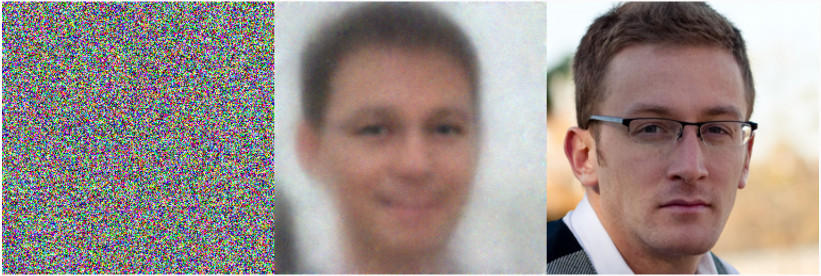
$t = 700$

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_0$

$t = 800$

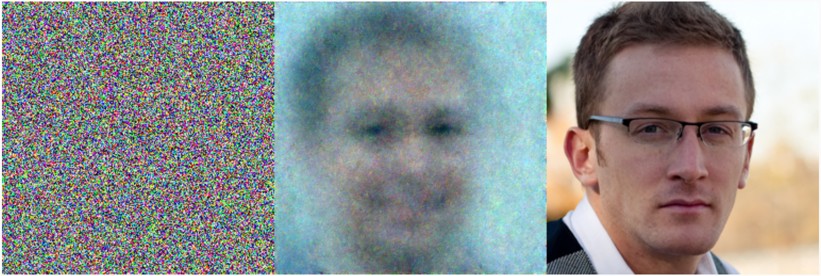
DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

We get the associated estimation of $\boldsymbol{x}_0$:

$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_0$

$t = 900$

DDPM: Denoiser

The Unet $\varepsilon_\theta(\boldsymbol{x}_t, t)$ is a (residual) denoiser that gives an estimation of the noise ε from

$$\boldsymbol{x}_t(\boldsymbol{x}_0, \boldsymbol{\varepsilon}) = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\varepsilon}.$$

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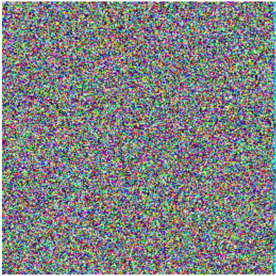
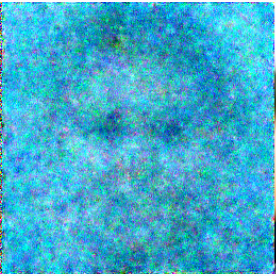
$$\hat{\boldsymbol{x}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\boldsymbol{x}_t - \sqrt{\frac{1}{\bar{\alpha}_t} - 1}\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t).$$



$\boldsymbol{x}_t$



$\hat{\boldsymbol{x}}_0$

$\boldsymbol{x}_0$

$t = 1000$

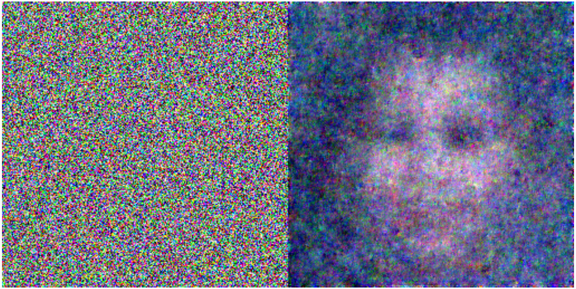
Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here. (source: (Ho et al., 2020))



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 999$

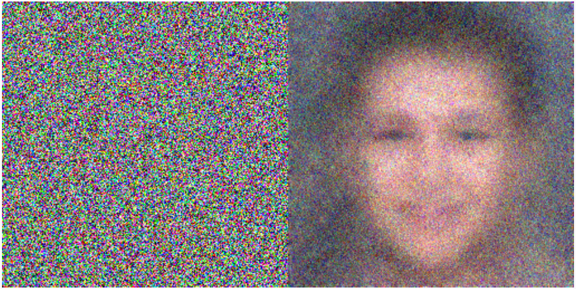
Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here. (source: (Ho et al., 2020))



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 900$

Algorithm 1 Training

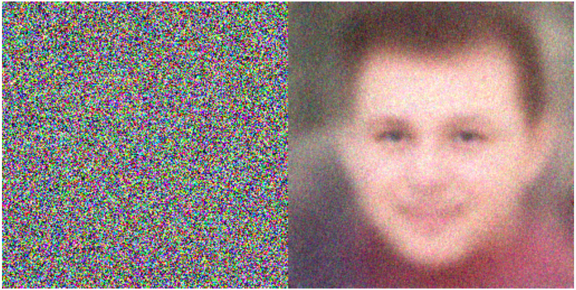
repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here.

(source: (Ho et al., 2020))



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 800$

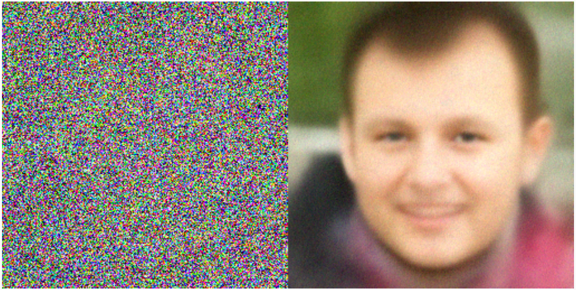
Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here. (source: (Ho et al., 2020))



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 700$

DDPM: Sampling

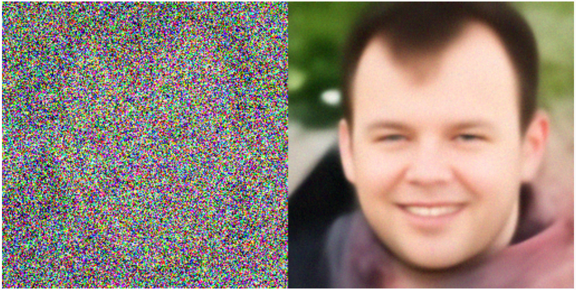
Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here. (source: (Ho et al., 2020))



$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 600$

DDPM: Sampling

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \text{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here.

(source: (Ho et al., 2020))

$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 500$

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here. (source: (Ho et al., 2020))

$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 400$

DDPM: Sampling

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here.

(source: (Ho et al., 2020))

$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 300$

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \text{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
  $$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here. (source: (Ho et al., 2020))

$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 200$

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here.

(source: (Ho et al., 2020))

$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 100$

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

$\sigma_t = \sqrt{\beta_t}$ here.

(source: (Ho et al., 2020))

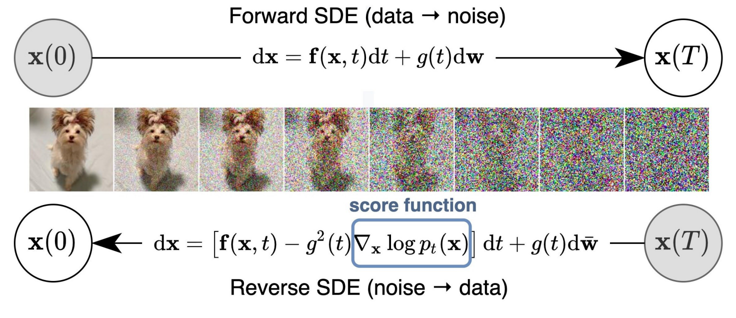
$\boldsymbol{x}_t$ $\hat{\boldsymbol{x}}_0$

$t = 0$

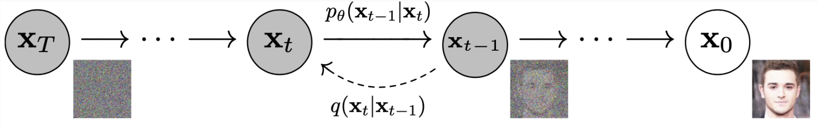
Continuous and discrete diffusion models

Recap on diffusion models

Diffusion model via SDE: (Song et al., 2021b)



Diffusion model via Denoising Diffusion Probabilistic Models (DDPM):
(Ho et al., 2020) Discrete model with a fixed number of $T = 10^3$.



Continuous diffusion models

Forward diffusion:

$$d\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_t, t)dt + g(t)d\boldsymbol{w}_t$$

Backward diffusion: $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$

$$d\boldsymbol{y}_t = \left[-\boldsymbol{f}(\boldsymbol{y}_t, T-t) + g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t)\right] dt + g(T-t)d\boldsymbol{w}_t.$$

- Learn score by denoising score matching:

$$\boxed{\theta^\star = \operatorname{argmin} \mathbb{E}_t \left(\lambda_t \mathbb{E}_{(\boldsymbol{x}_0, \boldsymbol{x}_t)} \|s_\theta(\boldsymbol{x}_t, t) - \nabla_{\boldsymbol{x}_t} \log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2\right)} \text{ with } t \sim \mathrm{Unif}([0, T])$$

- Generate samples by SDE discrete scheme (e.g. Euler-Maruyama):

$$\boldsymbol{Y}_{n-1} = \boldsymbol{Y}_n - h\boldsymbol{f}(\boldsymbol{Y}_n, t_n) + hg(t_n)^2 \boldsymbol{s}_\theta(\boldsymbol{Y}_n, t_n) + g(t_n)\sqrt{h}\boldsymbol{Z}_n \quad \text{with} \quad \boldsymbol{Z}_n \sim \mathcal{N}(\boldsymbol{0}, I_d)$$

- Associated deterministic probability flow:

$$d\boldsymbol{y}_t = \left[-\boldsymbol{f}(\boldsymbol{y}_t, T-t) + \frac{1}{2} g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t)\right] dt$$

Denoising Diffusion Probabilistic Models (DDPM)

Forward diffusion:

$$q(x_{0:T}) = \underbrace{q(\boldsymbol{x}_0)}_{\text{data distribution}} \prod_{t=1}^{T} \underbrace{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}_{\text{fixed forward transitions}} \quad \text{with} \quad q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}\boldsymbol{x}_{t-1}, \beta_t \boldsymbol{I}_d)$$

Backward diffusion: **stochastic decoder** p_θ:

$$p_\theta(\boldsymbol{x}_{0:T}) = \underbrace{p(\boldsymbol{x}_T)}_{\text{fixed latent prior}} \prod_{t=1}^{T} \underbrace{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}_{\text{learnt backward transitions}} \quad \text{with} \quad \underbrace{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) = \mathcal{N}(\mu_\theta(\boldsymbol{x}_t, t), \beta_t \boldsymbol{I}_d)}_{\text{Gaussian approximation of } q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}$$

- Learn the score by minimizing the ELBO (like for VAE): This boils down to denoising the diffusion iterations $\boldsymbol{x}_t = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\varepsilon}$:

$$\theta^\star = \operatorname{argmin} \sum_{t=1}^{T} \frac{\beta_t}{1-\bar{\alpha}_t} \mathbb{E}_q\left[\|\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t) - \boldsymbol{\varepsilon}\|^2\right] + C$$

- Sampling through the stochastic decoder with

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

DDPM training and score matching

Posterior mean training: Recall that $\mu_\theta(\boldsymbol{x}_t, t)$ minimizes

$$\mathbb{E}_q\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\|p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right] = \frac{1}{\beta_t}\mathbb{E}_q\left[\|\mu_\theta(\boldsymbol{x}_t,t) - \tilde{\mu}(\boldsymbol{x}_t,\boldsymbol{x}_0)\|^2\right] + C$$

where $\tilde{\mu}(\boldsymbol{x}_t, \boldsymbol{x}_0)$ is the mean of $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0)$. Hence ideally,

$$\mu_\theta(\boldsymbol{x}_t,t) = \mathbb{E}\left[\tilde{\mu}(\boldsymbol{x}_t,\boldsymbol{x}_0)|\boldsymbol{x}_t\right] = \mathbb{E}\left[\mathbb{E}\left[\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0\right]|\boldsymbol{x}_t\right] = \mathbb{E}\left[\boldsymbol{x}_{t-1}|\boldsymbol{x}_t\right].$$

Noise prediction training: $\varepsilon_\theta(\boldsymbol{x}_t, t)$ minimizes

$$\mathbb{E}_q\left[\|\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t,t) - \boldsymbol{\varepsilon}\|^2\right]$$

where ε is a function of $(\boldsymbol{x}_t, \boldsymbol{x}_0)$ (since $\boldsymbol{x}_t = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\varepsilon}$). Hence ideally,

$$\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t,t) = \mathbb{E}\left[\boldsymbol{\varepsilon}|\boldsymbol{x}_t\right]$$

Score matching training: Ideally,

$$s_\theta(\boldsymbol{x}_t,t) = \nabla_{\boldsymbol{x}_t}\log p_t(\boldsymbol{x}_t) = \mathbb{E}\left[\nabla_{\boldsymbol{x}_t}\log p_{t|0}(\boldsymbol{x}_t|\boldsymbol{x}_0)|\boldsymbol{x}_t\right]$$

Tweedie formulas

We derived the formulas for DDPM training without considering the score function... but denoising and score functions are linked by **Tweedie formulas**:

Theorem (Tweedie formulas)
If $\boldsymbol{Y} = a\boldsymbol{X} + \sigma \boldsymbol{Z}$ with $\boldsymbol{Z} \sim \mathcal{N}(\mathbf{0}, I_d)$ independent of $\boldsymbol{X}$, $a > 0$, $\sigma > 0$, then

Tweedie denoiser: $$\boxed{\mathbb{E}[\boldsymbol{X}|\boldsymbol{Y}] = \frac{1}{a}\left(\boldsymbol{Y} + \sigma^2 \nabla_{\boldsymbol{y}} \log p_{\boldsymbol{Y}}(\boldsymbol{Y})\right)}$$

Tweedie noise predictor: $$\boxed{\mathbb{E}[\boldsymbol{Z}|\boldsymbol{Y}] = -\sigma \nabla_{\boldsymbol{y}} \log p_{\boldsymbol{Y}}(\boldsymbol{Y})}$$

DDPM and Tweedie

If $Y = aX + \sigma Z$, **Tweedie denoiser:** $\mathbb{E}[X|Y] = \frac{1}{a}\left(Y + \sigma^2 \nabla_y \log p_Y(Y)\right)$

Tweedie noise predictor: $\mathbb{E}[Z|Y] = -\sigma \nabla_y \log p_Y(Y)$

Tweedie for noise prediction: Predict the noise ε from x_t:

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\varepsilon \quad \Rightarrow \quad \mathbb{E}\left[\varepsilon | x_t\right] = -\sqrt{1 - \bar{\alpha}_t} \nabla_{x_t} \log p_t(x_t)$$

Tweedie for one-step denoising: Predict x_{t-1} from x_t:

$$x_t = \sqrt{\alpha_t}\, x_{t-1} + \sqrt{\beta_t}\, z_t \quad \Rightarrow \quad \mathbb{E}[x_{t-1}|x_t] = \frac{1}{\sqrt{\alpha_t}}\left(x_t + \beta_t \nabla_{x_t} \log p_t(x_t)\right)$$

$$\mathbb{E}[x_{t-1}|x_t] = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \mathbb{E}\left[\varepsilon | x_t\right]\right)$$

DDPM and Tweedie

If $Y = aX + \sigma Z$, **Tweedie denoiser:** $$\mathbb{E}[X|Y] = \frac{1}{a}\left(Y + \sigma^2 \nabla_y \log p_Y(Y)\right)$$

Tweedie noise predictor: $$\mathbb{E}[Z|Y] = -\sigma \nabla_y \log p_Y(Y)$$

Tweedie for noise prediction: Predict the noise ε from x_t:

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\varepsilon \quad \Rightarrow \quad \mathbb{E}\left[\varepsilon | x_t\right] = -\sqrt{1-\bar{\alpha}_t}\nabla_{x_t} \log p_t(x_t)$$

Tweedie for one-step denoising: Predict x_{t-1} from x_t:

$$x_t = \sqrt{\alpha_t}\, x_{t-1} + \sqrt{\beta_t}\, z_t \quad \Rightarrow \quad \mathbb{E}[x_{t-1}|x_t] = \frac{1}{\sqrt{\alpha_t}}\left(x_t + \beta_t \nabla_{x_t} \log p_t(x_t)\right)$$

$$\mathbb{E}[x_{t-1}|x_t] = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\mathbb{E}\left[\varepsilon | x_t\right]\right)$$

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t, t)\right)$$

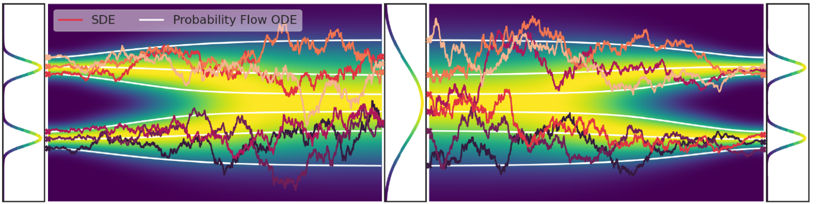
Remarks: We recover the expression of $\mu_\theta(x_t, t)$ without using the one of

$$\tilde{\mu}(x_t, x_0) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon\right)$$

DDPM and score matching

To sum up:

- The three trainings strategies are the same (up to weighting constants).
- The only difference between the continuous SDE model and the discrete DDPM model are the time values: $t \in [0, T]$ VS. $t = 1, \dots, T = 10^3$.
- **Good news:** We can train a DDPM and use it for a deterministic probability flow ODE (this is what is done by the DDIM model (Song et al., 2021a)).



(source: (Song and Ermon, 2020))

Diffusion models for imaging inverse problems

Diffusion posterior sampling

We present **Diffusion Posterior Sampling (DPS)** for general noisy inverse problems (Chung et al., 2023)

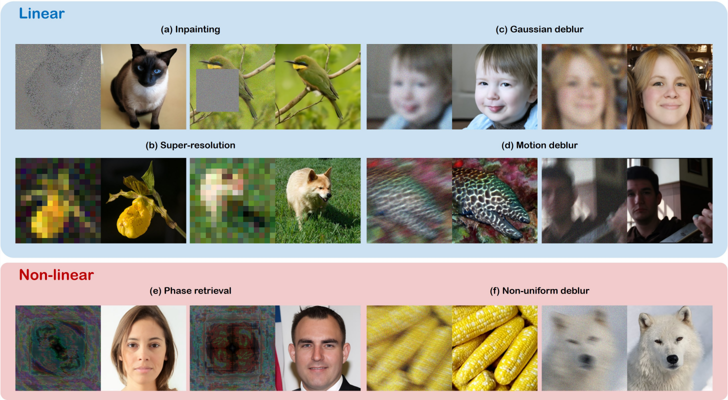


Figure 1: Solving noisy linear, and nonlinear inverse problems with diffusion models. Our reconstruction results (right) from the measurements (left) are shown.

(source: (Chung et al., 2023))

See also (Song et al., 2023), (Kawar et al., 2022) for alternative methods.

Conditional sampling

Let A be a linear operator from an inverse problem (masking operator for inpainting, blur operator for deblurring, subsampling for SR, ...).

Given some observation

$$\boldsymbol{y} = A\boldsymbol{x}_{\text{unknown}} + \boldsymbol{n}$$

where $\boldsymbol{n}$ is some additive white Gaussian noise with variance σ^2, we would like to sample

$$p_0(\boldsymbol{x}_0 | A\boldsymbol{x}_0 + \boldsymbol{n} = \boldsymbol{y}) = p_0(\boldsymbol{x}_0 | \boldsymbol{y})$$

to estimate $\boldsymbol{x}_{\text{unknown}}$ in accordance with the prior of the generative model.

Conditional sampling

From (Song et al., 2021b), we can consider the SDE for the conditional distribution $p_0(\boldsymbol{x}_0|\boldsymbol{y})$:

Backward diffusion for VP-SDE: $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$

$$d\boldsymbol{y}_t = [\beta_{T-t}\boldsymbol{y}_t + \beta_{T-t}\nabla_{\boldsymbol{x}=\boldsymbol{y}_t} \log p_{T-t}(\boldsymbol{y}_t)]\, dt + \beta_{T-t} d\boldsymbol{w}_t.$$

Conditional backward diffusion for VP-SDE: $\boldsymbol{y}_t = \boldsymbol{x}_{T-t}$

$$d\boldsymbol{y}_t = [\beta_{T-t}\boldsymbol{y}_t + \beta_{T-t}\nabla_{\boldsymbol{x}=\boldsymbol{y}_t} \log p_{T-t}(\boldsymbol{y}_t|\boldsymbol{y})]\, dt + \beta_{T-t} d\boldsymbol{w}_t.$$

By Bayes rule:

$$\log p_{T-t}(\boldsymbol{y}_t|\boldsymbol{y}) = \log p_{T-t}(\boldsymbol{y}|\boldsymbol{y}_t) + \log(p_{T-t}(\boldsymbol{y}_t)) - \log(p_{T-t}(\boldsymbol{y}))$$

Thus,

$$\nabla_{\boldsymbol{x}=\boldsymbol{y}_t} \log p_{T-t}(\boldsymbol{y}_t|\boldsymbol{y}) = \underbrace{\nabla_{\boldsymbol{x}=\boldsymbol{y}_t} \log p_{T-t}(\boldsymbol{y}|\boldsymbol{y}_t)}_{\text{intractable}} + \underbrace{\nabla_{\boldsymbol{x}=\boldsymbol{y}_t} \log(p_{T-t}(\boldsymbol{y}_t))}_{\text{usual score function}}$$

For clarity, let us write the new term with forward notation:

$$\nabla_{\boldsymbol{x}=\boldsymbol{y}_t} \log p_{T-t}(\boldsymbol{y}|\boldsymbol{y}_t) = \nabla_{\boldsymbol{x}=\boldsymbol{x}_t} \log p_t(\boldsymbol{y}|\boldsymbol{x}_t)$$

Conditional sampling

(Chung et al., 2023) propose the following approximation:

$$\log p_t(\boldsymbol{y}|\boldsymbol{x}_t) \approx \log p_t(\boldsymbol{y}|\boldsymbol{x}_0 = \hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t))$$

with $\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t)$ the estimate of the original image from the network.

Since

$$p(\boldsymbol{y}|\boldsymbol{x}_0) = \frac{1}{(2\pi\sigma^2)^{\frac{n}{2}}} \exp\left(-\frac{\|\boldsymbol{y} - A\boldsymbol{x}_0\|^2}{2\sigma^2}\right)$$

we finally approximate

$$\nabla_{\boldsymbol{x}=\boldsymbol{x}_t} \log p_t(\boldsymbol{y}|\boldsymbol{x}_t) = -\frac{1}{2\sigma^2} \nabla_{\boldsymbol{x}_t} \|\boldsymbol{y} - A\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t)\|^2$$

- Computing $\nabla_{\boldsymbol{x}_t} \|\boldsymbol{y} - A\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t)\boldsymbol{x}_0\|^2$ involves a backpropagation through the Unet.
- One can expect this approximate conditional sampling to be twice as long as the sampling procedure.

Diffusion posterior sampling

Algorithm 1 DPS - Gaussian

Require: $N, \boldsymbol{y}, \{\zeta_i\}_{i=1}^N, \{\tilde{\sigma}_i\}_{i=1}^N$

$\boldsymbol{x}_N \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$
for $i = N-1$ **to** 0 **do**
  $\hat{\boldsymbol{s}} \leftarrow \boldsymbol{s}_\theta(\boldsymbol{x}_i, i)$
  $\hat{\boldsymbol{x}}_0 \leftarrow \frac{1}{\sqrt{\bar{\alpha}_i}}(\boldsymbol{x}_i + (1-\bar{\alpha}_i)\hat{\boldsymbol{s}})$
  $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$
  $\boldsymbol{x}'_{i-1} \leftarrow \frac{\sqrt{\alpha_i}(1-\bar{\alpha}_{i-1})}{1-\bar{\alpha}_i}\boldsymbol{x}_i + \frac{\sqrt{\bar{\alpha}_{i-1}}\beta_i}{1-\bar{\alpha}_i}\hat{\boldsymbol{x}}_0 + \tilde{\sigma}_i\boldsymbol{z}$
  $\boldsymbol{x}_{i-1} \leftarrow \boldsymbol{x}'_{i-1} - \zeta_i \nabla_{\boldsymbol{x}_i} \|\boldsymbol{y} - \mathcal{A}(\hat{\boldsymbol{x}}_0)\|_2^2$
end for
return $\hat{\mathbf{x}}_0$

(source: (Chung et al., 2023))

- Usual DDPM sampling (notation with $\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t)$ instead of $\varepsilon_\theta(\boldsymbol{x}_t, t)$.

$$\mu_\theta(\boldsymbol{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\boldsymbol{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(\boldsymbol{x}_t, t)\right) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\boldsymbol{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t)$$

- Add a correction term to drive $A\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t)$ close to $\boldsymbol{y}$.
- In practice $\zeta_i = \zeta_t \propto \|\boldsymbol{y} - A\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t, t)\|^{-1}$.

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

x_{unknown} y $\hat{x}_0$ x_t

$t = 999$

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 900$

Diffusion posterior sampling: Results

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 800$

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 700$

Diffusion posterior sampling: Results

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 600$

Diffusion posterior sampling: Results

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 500$

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 400$

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 300$

Diffusion posterior sampling: Results

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 200$

Diffusion posterior sampling: Results

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 100$

- Very good results in terms of perceptual metric (LPIPS).

Inpainting:

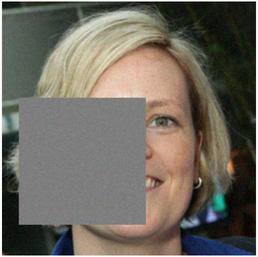
$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 0$

Diffusion posterior sampling: Inpainting results

- Very good results in terms of perceptual metric (LPIPS).
- Lack of symmetry.
- It can sometimes be really bad though!

original $\boldsymbol{x}_{\text{unknown}}$



input $\boldsymbol{y}$

output $\boldsymbol{x}_0$

Diffusion posterior sampling: Inpainting results

- Very good results in terms of perceptual metric (LPIPS).
- Lack of symmetry.
- It can sometimes be really bad though!


original $\boldsymbol{x}_{\text{unknown}}$


input $\boldsymbol{y}$


output $\boldsymbol{x}_0$

Diffusion posterior sampling: Inpainting results

- Very good results in terms of perceptual metric (LPIPS).
- Lack of symmetry.
- It can sometimes be really bad though!

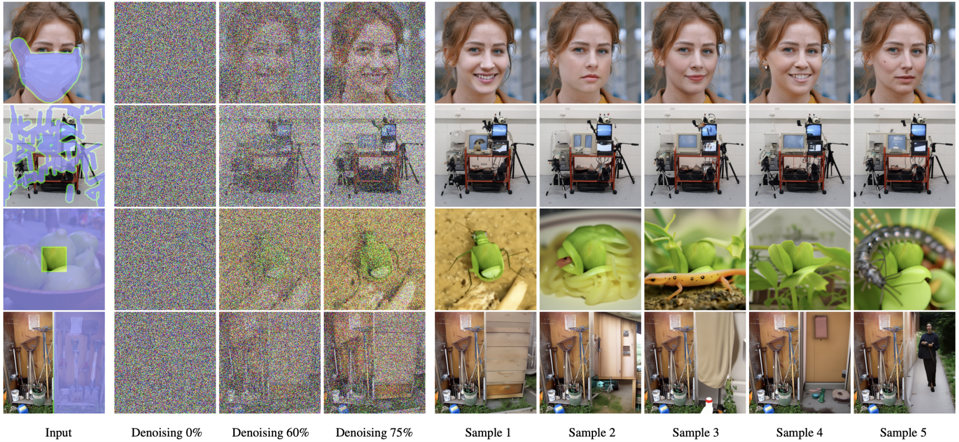
original $\boldsymbol{x}_{\text{unknown}}$

input $\boldsymbol{y}$

output $\boldsymbol{x}_0$

Diffusion posterior sampling: Inpainting results

- For inpainting it can help to go back and forth in the diffusion process (Lugmayr et al., 2022).



(source: (Lugmayr et al., 2022))

Diffusion posterior sampling: Super-resolution results

- Super-resolution with a factor $\times 4$.
- Very good results in terms of perceptual metric (LPIPS).
- Loss of details (skin defaults, etc.).

original $\boldsymbol{x}_{\text{unknown}}$

input $\boldsymbol{y}$

output $\boldsymbol{x}_0$

Diffusion posterior sampling: Super-resolution results

- Super-resolution with a factor $\times 4$.
- Very good results in terms of perceptual metric (LPIPS).
- Loss of details (skin defaults, etc.).

original $\boldsymbol{x}_{\text{unknown}}$

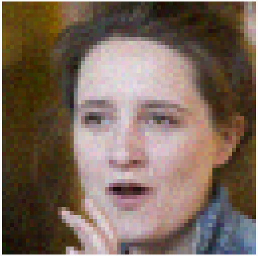
input $\boldsymbol{y}$

output $\boldsymbol{x}_0$

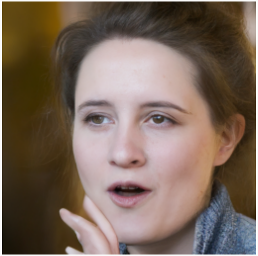
Diffusion posterior sampling: Super-resolution results

- Super-resolution with a factor $\times 4$.
- Very good results in terms of perceptual metric (LPIPS).
- Loss of details (skin defaults, etc.).

original $\boldsymbol{x}_{\text{unknown}}$



input $\boldsymbol{y}$



output $\boldsymbol{x}_0$

Conditional DDPM for super-resolution

- Super-resolution is often used to improve the quality of generated images.
- One can train a specific DDPM for this task by conditioning the Unet with the low resolution image $\varepsilon_\theta(\boldsymbol{x}_t, \boldsymbol{y}_{\mathrm{LR}}, t)$.

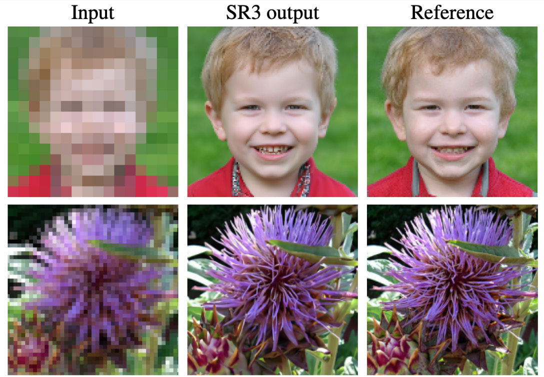
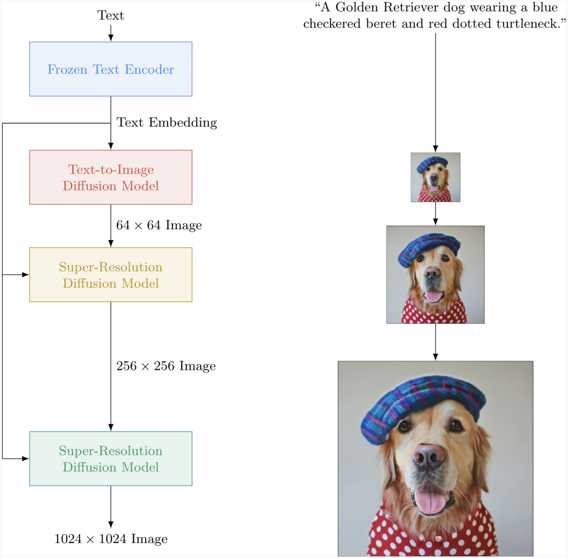


Figure 1: Two representative SR3 outputs: (top) 8× face super-resolution at 16×16→128×128 pixels (bottom) 4× natural image super-resolution at 64×64→256×256 pixels.

From (Saharia et al., 2023):
"To condition the model on the input $\boldsymbol{y}_{\mathrm{LR}}$, we upsample the low-resolution image to the target resolution using bicubic interpolation. The result is concatenated with $\boldsymbol{x}_t$ along the channel dimension."

Conditional DDPM for super-resolution

Imagen pipeline:
Text conditioning
&
Conditional
super-resolution
via DDPM



(source: (Saharia et al., 2022))

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