Introduction to diffusion models

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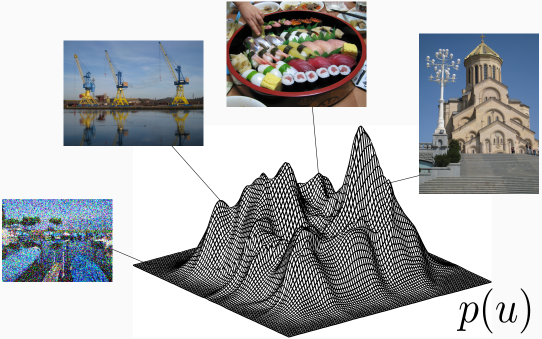
Material for the course is here:
https://www.idpoisson.fr/galerne/hk2024/index.html

Introduction on generative models

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



(source: Charles Deledalle)

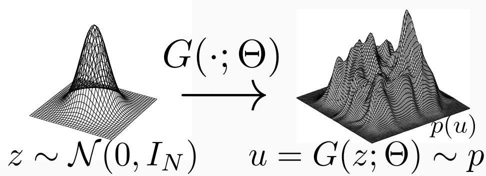
The images may represent:

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

2. Generate samples from this distribution.

Generative models

1. Model and/or learn a distribution $p(u)$ on the space of images.
2. Generate samples from this distribution.



- 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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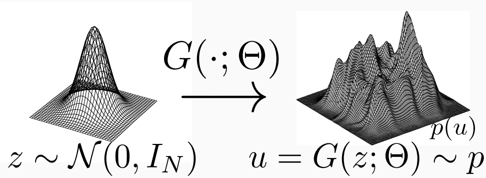


- z is a generic source of randomness, often called the latent variable.
- If $G(\cdot;\Theta)$ is known, then $p = G(\cdot;\Theta)_{\#}\mathcal{N}(0, I_n)$ is the push-forward of the latent distribution.

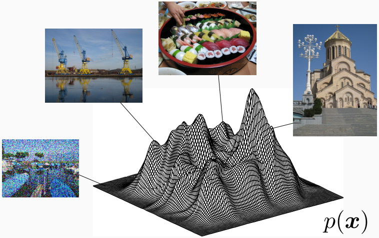
The generator $G(\cdot;\Theta)$ can be:

- 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,...).

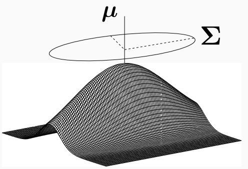
- Consider a **Gaussian model** for the distribution of images $\boldsymbol{x}$ with d pixels:

$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}|}} \exp\left[-(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\right]$$

  - $\boldsymbol{\mu}$: mean image,
  - $\boldsymbol{\Sigma}$: covariance matrix of images.



$\approx$



Gaussian prior $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

(source: Charles Deledalle)

Image generation: Gaussian model

- Take a training dataset $\mathcal{D}$ of images:

$$\mathcal{D} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$$

$$= \Big\{ \dots \Big\}_{\times N}$$

- Estimate the mean

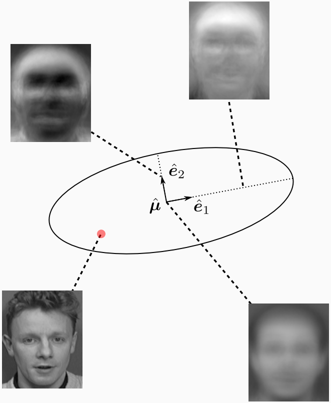
$$\hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_i \boldsymbol{x}_i =$$

- Estimate the covariance matrix: $\hat{\boldsymbol{\Sigma}} = \frac{1}{N} \sum_i (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})^T = \hat{\boldsymbol{E}} \hat{\boldsymbol{\Lambda}} \hat{\boldsymbol{E}}^T$

$$\hat{\boldsymbol{E}} = \underbrace{\Big\{ \dots \Big\}_{\times N}}_{\text{eigenvectors of } \hat{\boldsymbol{\Sigma}},\ \textit{i.e.}\text{, main variation axis}}$$

Image generation: Gaussian model

You now have learned a **generative model**:



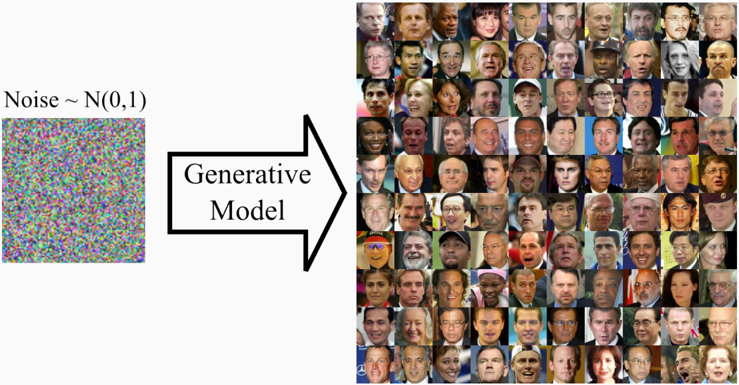
How to generate samples from $\mathcal{N}(\hat{\mu}, \hat{\Sigma})$?

$$\begin{cases} z & \sim \mathcal{N}(0, I_d) \quad \leftarrow \text{Generate random latent variable} \\ x & = \hat{\mu} + \hat{E}\hat{\Lambda}^{1/2} z \end{cases}$$

The model does not generate realistic faces.

- The Gaussian distribution assumption is too simplistic.
- Each generated image is just a linear random combination of the eigenvectors (with independence !).
- The generator corresponds to a one layer liner neural network (without non-linearities).

Image generation: Gaussian model



- Deep generative modeling consists in learning non-linear generative models to reproduce complex data such as realistic images.
- It relies on deep neural networks and several solutions have been proposed since the “Deep learning revolution” (2012).

Texture synthesis with a stationary Gaussian model: (Galerne et al., 2011)

- Data: A single texture image $\boldsymbol{h}$.
- Inferred distribution: p is the stationary Gaussian distribution with similar mean and covariance statistics.
- z is a Gaussian white noise image (each pixel is iid with standard normal distribution).
- G is a convolution operator with know parameters Θ.

Data | Generated images

Spot $\boldsymbol{h}$

$G(z_1; \Theta)$

$G(z_2; \Theta)$

$G(z_3; \Theta)$

Generative models: Examples

Generative Adversarial Networks: (Goodfellow et al., 2014)

- Data: A database of images.
- Inferred distribution: Not explicit, push-forward measure given by generator.
- z is a Gaussian array in a latent space.
- $G(\cdot;\Theta)$ is a (convolutional) neural network with parameters Θ learned using an adversarial discriminator network $D(\cdot;\Theta_D)$.

Data

MNIST: handwritten digits

Generated images

Fake images (100 epochs)

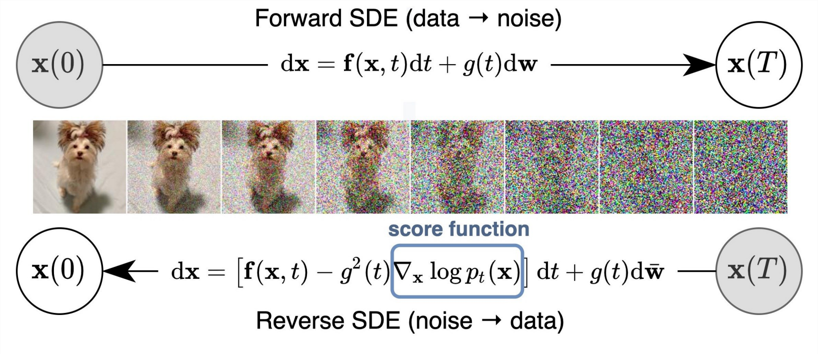
Image size: 28×28 px

Generative Adversarial Networks: Style GAN (Karras et al., 2019)

Image size:
1024$\times$ 1024 px
(source: Karras et al.)

Denoising diffusion probabilistic models

- Learn to revert a degradation process: Add more and more noise to an image.
- First similar model (Sohl-Dickstein et al., 2015)



(source: Yang Song)

- Probably the most promising framework these days... but things change very quickly in this field!

(Ho et al., 2020): Denoising Diffusion Probabilistic Models (DDPM): One of the first paper producing images with reasonable resolution.

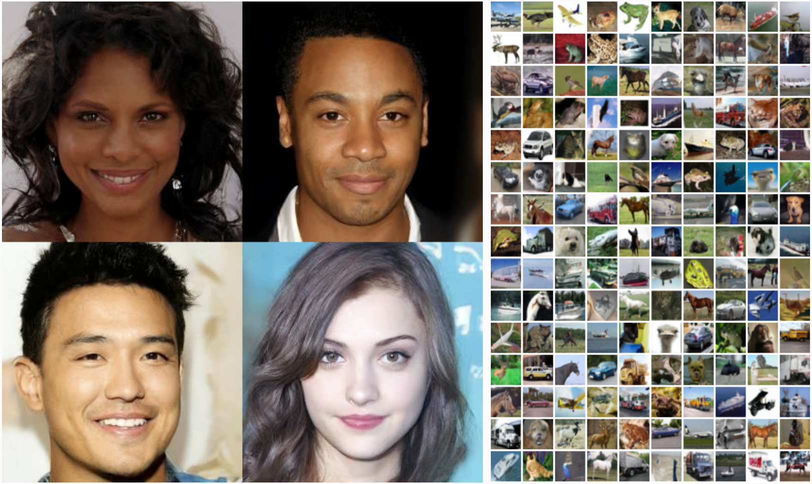


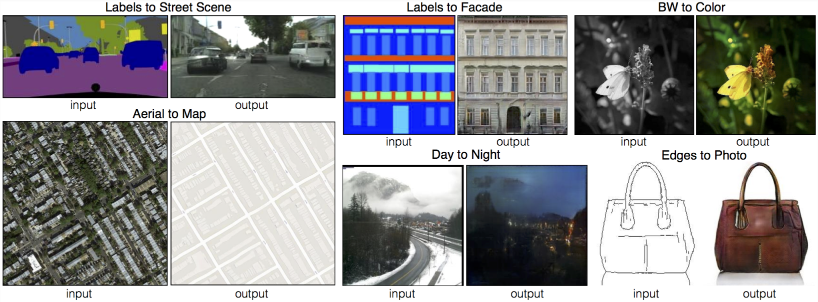
Figure 1: Generated samples on CelebA-HQ 256×256 (left) and unconditional CIFAR10 (right)

Generative models: Motivations

Why generative models are interesting ?

- **Generating realistic images is important by itself** for entertainment industry (visual effects, video games, augmented reality...), design, advertising industry,...
- **Good image model leads to good image processing:** Generative models can be used as a parametric space for solving inverse problems. Example: Inpainting of a portrait image.
- Also generative models opens the way to **non trivial image manipulation** using **conditional generative models**.

Pix2pix: Image-to-Image Translation with Conditional Adversarial Nets (Isola et al., 2017)



- GAN conditioned on input image.
- Generator: U-net architecture
- Discriminator: Patch discriminator applied to each patch
- Opens the way for new creative tools

(source: Isola et al.)

Conditional generative models: Examples

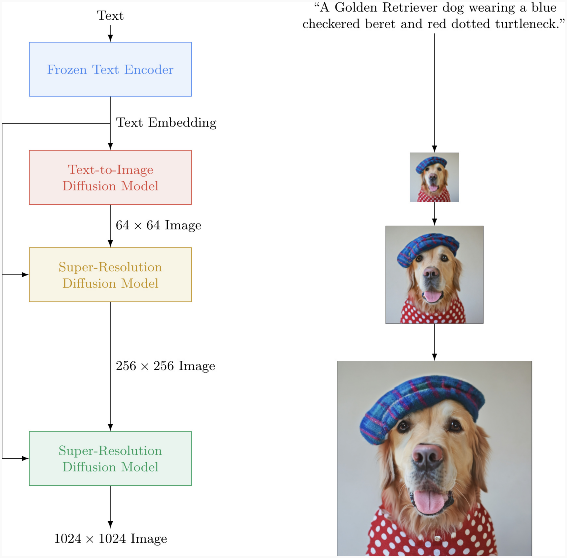
Latest trends using **diffusion models**: Text to image generation

- DALL·E 1 & 2: CreatingImages from Text (Open AI, January 2021 and April 2022)
- Imagen, Google research (May 2022)

DALL·E 2 (Open AI)
Input: An astronaut riding a horse in a photorealistic style

Imagen (Google)
Input: A dog looking curiously in the mirror, seeing a cat.

Imagen pipeline:



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

In August 2022, StableDiffusion was released:

- Based on the paper (Rombach et al., 2022)
- **Open source!**

futuristic tree house, hyper realistic, epic composition, cinematic, landscape vista photography by Carr Clifton & Galen Rowell, Landscape veduta photo by Dustin Lefevre & tdraw, detailed landscape painting by Ivan Shishkin, rendered in Enscape, Miyazaki, Nausicaa Ghibli, 4k detailed post processing, unreal engine
Steps: 50, Sampler: PLMS, CFG scale: 9, Seed: 2937258437

Diffusion models in 2023

Diffusion models are considered mature models and have been used in a large variety of frameworks.

- Diffusion models **beyond image generation**: Text to video, motion generation, proteins, soft robots,...
- **Control of (latent) diffusion models**((Ruiz et al., 2023), (Zhang et al., 2023),...)
- **Diffusion models as priors for imaging inverse problems** ((Chung et al., 2023), (Song et al., 2023), lot of applications in medical imaging, etc.)

Diffusion models in 2023

DreamBooth: Fine Tuning Text-to-Image Diffusion Models for Subject-Driven Generation

Nataniel Ruiz*[1,2] Yuanzhen Li[1] Varun Jampani[1]
Yael Pritch[1] Michael Rubinstein[1] Kfir Aberman[1]
[1] Google Research [2] Boston University

Figure 1. With just a few images (typically 3-5) of a subject (left), *DreamBooth*—our AI-powered photo booth—can generate a myriad of images of the subject in different contexts (right), using the guidance of a text prompt. The results exhibit natural interactions with the environment, as well as novel articulations and variation in lighting conditions, all while maintaining high fidelity to the key visual features of the subject.

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

Adding Conditional Control to Text-to-Image Diffusion Models

Lvmin Zhang, Anyi Rao, and Maneesh Agrawala
Stanford University
{lvmin, anyirao, maneesh}@cs.stanford.edu

Input Canny edge | Default | "masterpiece of fairy tale, giant deer, golden antlers" | "..., quaint city Galic"

Input human pose | Default | "chef in kitchen" | "Lincoln statue"

Figure 1: Controlling Stable Diffusion with learned conditions. ControlNet allows users to add conditions like Canny edges (top), human pose (bottom), *etc.*, to control the image generation of large pretrained diffusion models. The default results use the prompt "a high-quality, detailed, and professional image". Users can optionally give prompts like the "chef in kitchen".

(source: ControlNet (Zhang et al., 2023))

Diffusion posterior sampling for general noisy inverse problems (Chung et al., 2023)

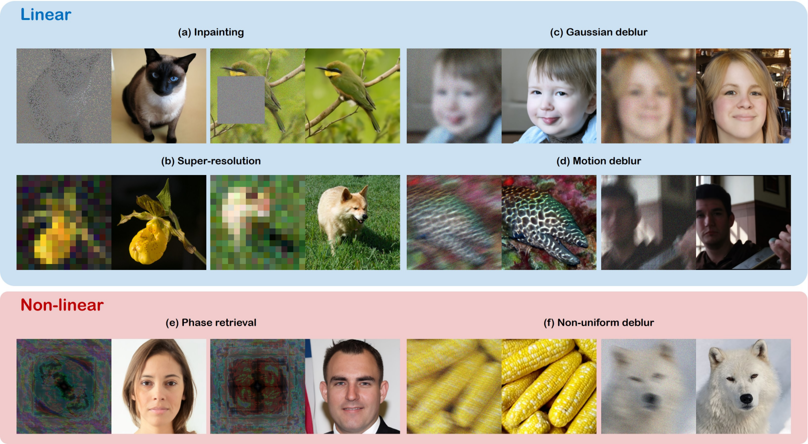


Figure 1: Solving noisy linear, and nonlinear inverse problems with diffusion models. Our reconstruction results (right) from the measurements (left) are shown.

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

1. Introduction to generative models for images (done)
2. Basics on diffusion models: Continuous and discrete formulation
3. Diffusion models for imaging inverse problems

Basics on diffusion models

Adding noise to images

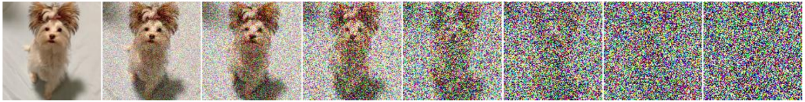
- We are given an input dataset

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

- 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,

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

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

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

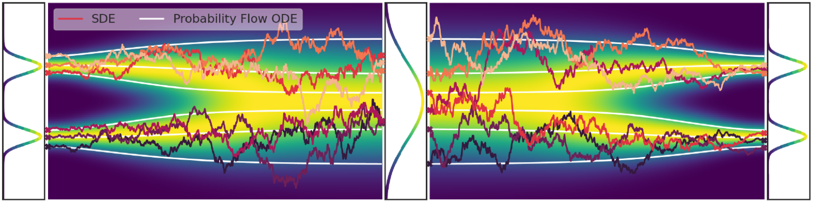
$$\boldsymbol{X}_{n+1} = \boldsymbol{X}_n + \boldsymbol{f}(\boldsymbol{X}_n, t_n)h + g(t_n)\left(\boldsymbol{w}_{t_{n+1}} - \boldsymbol{w}_{t_n}\right), \quad n = 1, \dots, N-1.$$

- 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

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

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...).

Reversed diffusion

Forward diffusion:

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

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

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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:

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

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

$$\boxed{\nabla_{x_t} \log p_t(x_t) = \mathbb{E}_{x_0 \sim p_{0|t}(x_0|x_t)} \left[\nabla_{x_t} \log p_{t|0}(x_t|x_0) \right] = \mathbb{E}\left[\nabla_{x_t} \log p_{t|0}(x_t|x_0) | x_t \right]}$$

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 $x_t \mapsto \nabla_{x_t} \log p_t(x_t)$ is the solution

$$\boxed{\nabla_{x_t} \log p_t = \operatorname{argmin}\{\mathbb{E}_{p_{0,t}} \|f(x_t) - \nabla_{x_t} \log p_{t|0}(x_t|x_0)\|^2,\ f \in \mathrm{L}^2(p_t)\}}$$

- We obtain a **loss function** to learn the function f using Monte Carlo approximation with samples (x_0, x_t) for the expectation.

Learning the score function: Denoising score matching

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

- $f : \mathbb{R}^d \to \mathbb{R}^d$ 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)

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

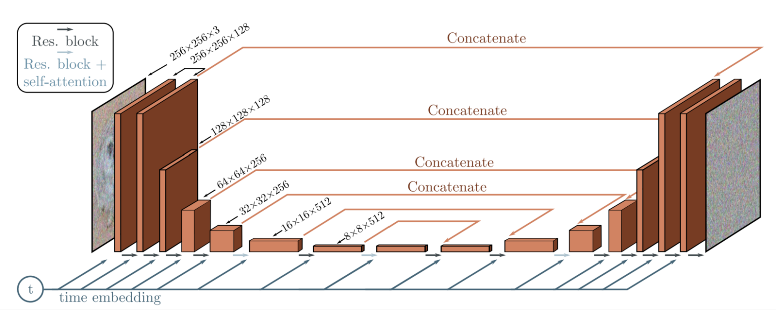
where t is chosen uniformly in $[0, T]$ and $t \mapsto \lambda_t$ is a weighting term to balance the importance of each t.

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).

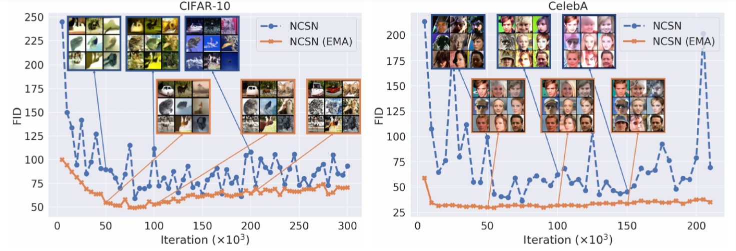


(source: learnopencv.com)

- 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.

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

- 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):

$$X_{n+1} = X_n + \gamma \nabla_x \log p(X_n) + \sqrt{2\gamma} Z_n$$

- (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 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:

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

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

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

Sampling via an ODE

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

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&= \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:

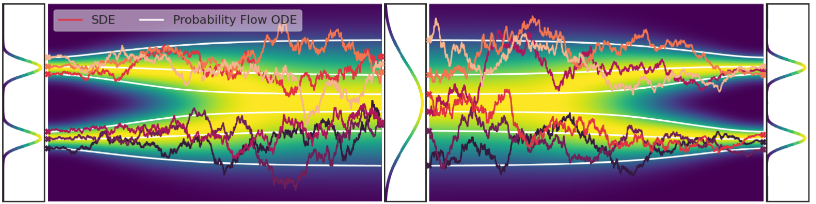
$$d\boldsymbol{y}_t = \left[-\boldsymbol{f}(\boldsymbol{y}_t, T-t) + \frac{1}{2} g(T-t)^2 \nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{y}_t)\right] dt.$$

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

Reverse diffusion via an ODE

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

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



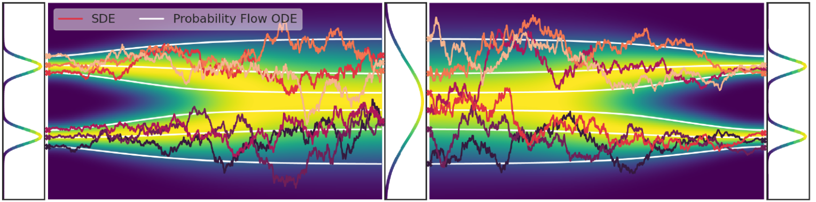
(source: (Song and Ermon, 2020))

- 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

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

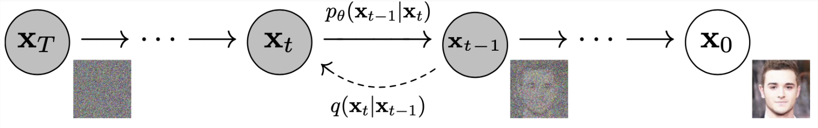
This ODE is called a **probability flow ODE**.



(source: (Song and Ermon, 2020))

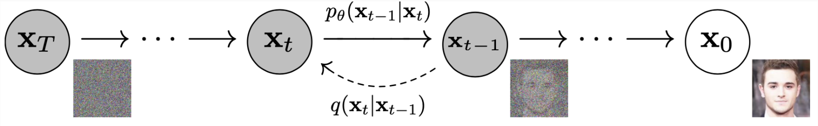
- From (Karras et al., 2022) "Through extensive tests, we have found Heun's 2nd order method (a.k.a. improved Euler, trapezoidal rule) [...] to provide an excellent tradeoff between truncation error and NFE."
- Requires much less NFE than stochastic samplers (eg around 50 steps instead of 1000), see 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: $q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}\boldsymbol{x}_{t-1}, \beta_t I_d)$

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

  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:

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

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

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

- 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**.

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

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

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$= \dots$ (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)

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

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,

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

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

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

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

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

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

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

- 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

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

Algorithm 2 Sampling

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

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

$\boldsymbol{x}_t$

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

$\boldsymbol{x}_0$

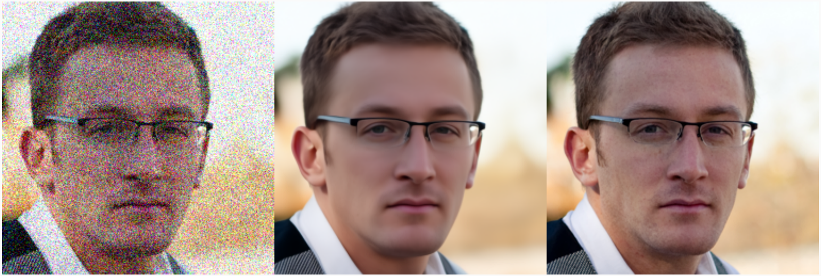
$t = 11$

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 $\boldsymbol{x}_0$:

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



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

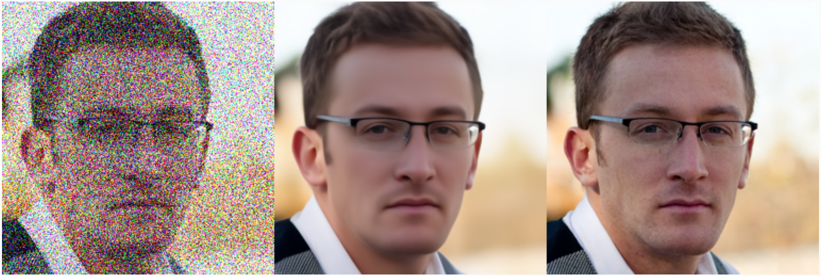
$t = 100$

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 $\boldsymbol{x}_0$:

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



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

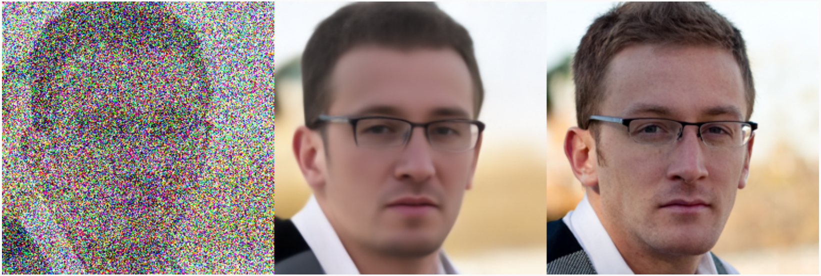
$t = 200$

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 $\boldsymbol{x}_0$:

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



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

$t = 400$

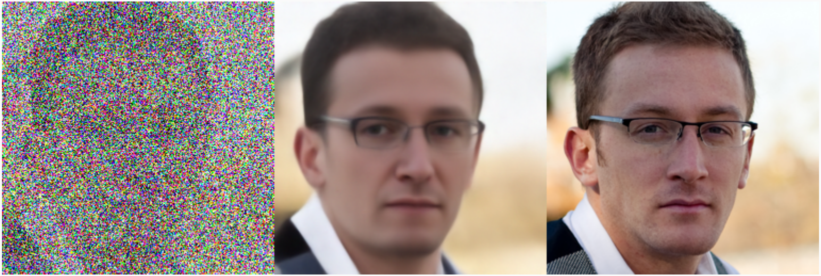
DDPM: Denoiser

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 $\boldsymbol{x}_0$:

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



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

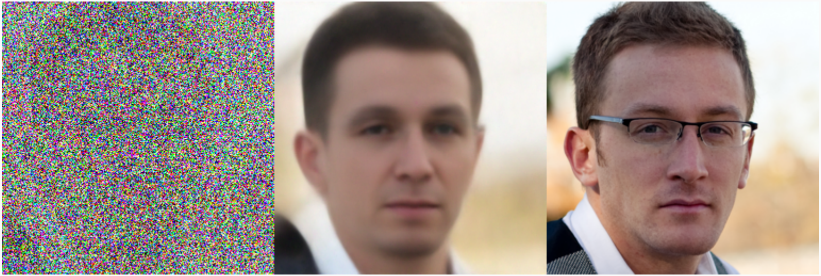
$t = 500$

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 $\boldsymbol{x}_0$:

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



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

$t = 600$

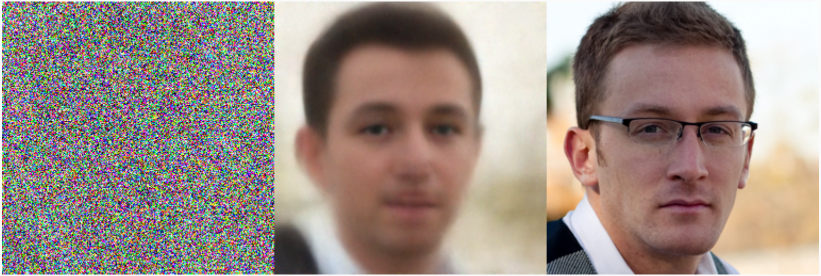
DDPM: Denoiser

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 $\boldsymbol{x}_0$:

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



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

$t = 700$

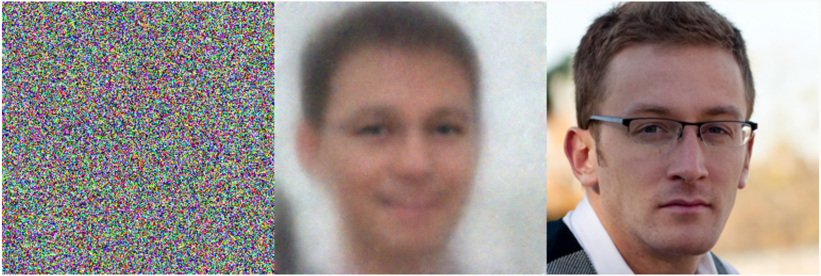
DDPM: Denoiser

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 $\boldsymbol{x}_0$:

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



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

$t = 800$

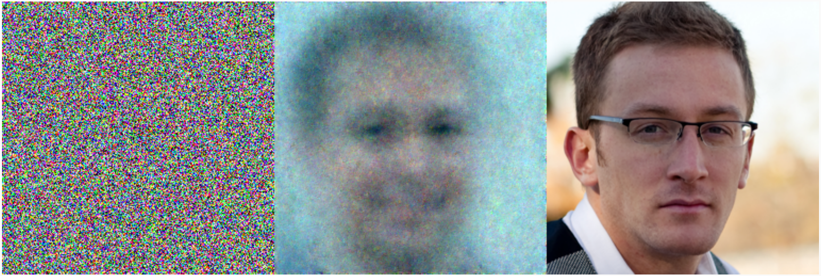
DDPM: Denoiser

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 $\boldsymbol{x}_0$:

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



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

$t = 900$

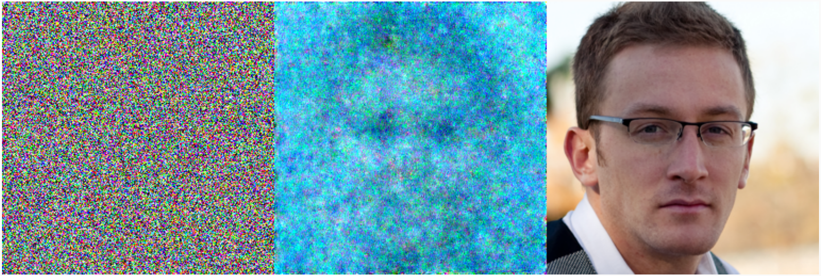
DDPM: Denoiser

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

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

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

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



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

$t = 1000$

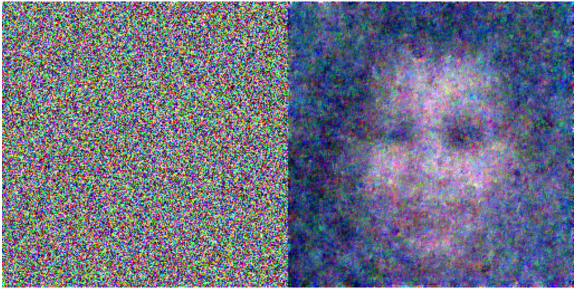
Algorithm 1 Training

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

Algorithm 2 Sampling

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

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



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

$t = 999$

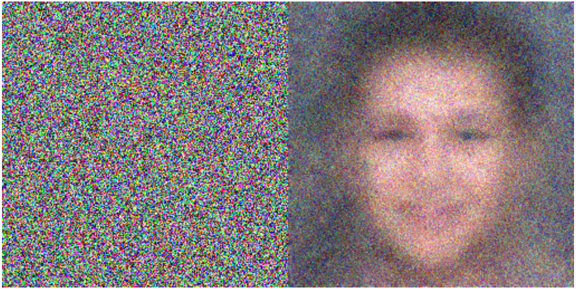
Algorithm 1 Training

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

Algorithm 2 Sampling

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

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



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

$t = 900$

DDPM: Sampling

Algorithm 1 Training

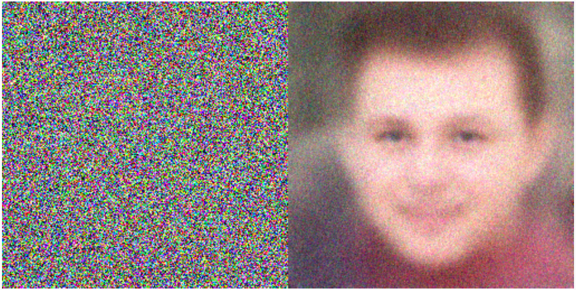
1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0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

Algorithm 2 Sampling

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

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

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



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

$t = 800$

DDPM: Sampling

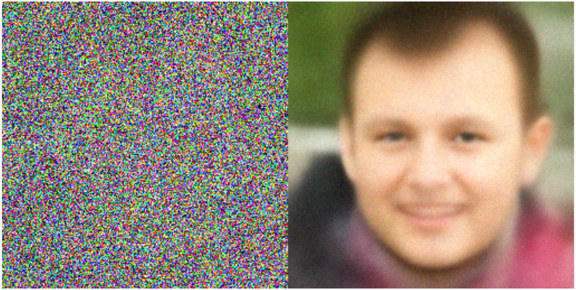
Algorithm 1 Training

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

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
5: **end for**
6: **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

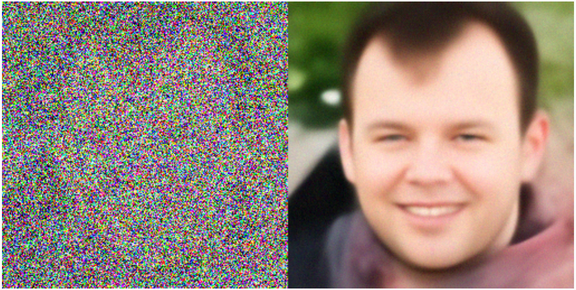
Algorithm 1 Training

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))



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

$t = 600$

Algorithm 1 Training

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

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
5: **end for**
6: **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
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  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))

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

$t = 400$

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

Algorithm 2 Sampling
1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

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

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

$t = 300$

DDPM: Sampling

Algorithm 1 Training

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

Algorithm 2 Sampling

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

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

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

$t = 200$

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))

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

$t = 100$

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 $\mathbf{x}_0$

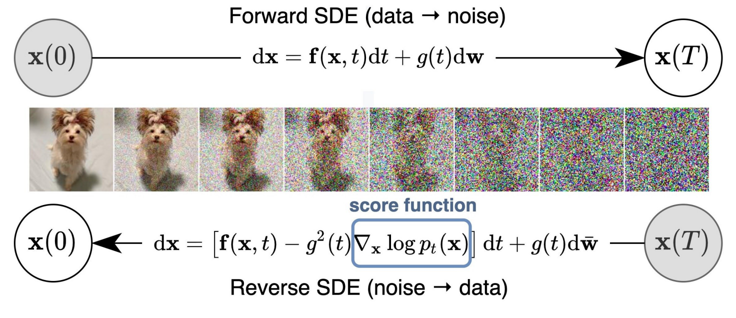
$\sigma_t = \sqrt{\beta_t}$ here. (source: (Ho et al., 2020))

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

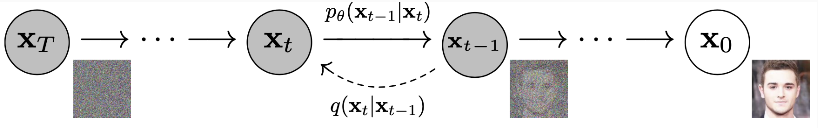
$t = 0$

Continuous and discrete 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:

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

Backward diffusion: **stochastic decoder** p_θ:

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

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

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

- 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: $\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t,t)$ minimizes

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

where $\boldsymbol{\varepsilon}$ 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 $\boldsymbol{Z} \sim \mathcal{N}(\boldsymbol{0}, I_d)$ 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: $$\boxed{\mathbb{E}[\boldsymbol{Z}|\boldsymbol{Y}] = -\sigma \nabla_{\boldsymbol{y}} \log p_{\boldsymbol{Y}}(\boldsymbol{Y})}$$

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

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

Tweedie for noise prediction: Predict the noise ε from $\boldsymbol{x}_t$:

$$\boldsymbol{x}_t = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\varepsilon} \quad \Rightarrow \quad \boxed{\mathbb{E}\left[\boldsymbol{\varepsilon}|\boldsymbol{x}_t\right] = -\sqrt{1-\bar{\alpha}_t}\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t)}$$

Tweedie for one-step denoising: Predict $\boldsymbol{x}_{t-1}$ from $\boldsymbol{x}_t$:

$$\boldsymbol{x}_t = \sqrt{\alpha_t}\,\boldsymbol{x}_{t-1} + \sqrt{\beta_t}\,\boldsymbol{z}_t \quad \Rightarrow \quad \mathbb{E}[\boldsymbol{x}_{t-1}|\boldsymbol{x}_t] = \frac{1}{\sqrt{\alpha_t}}\left(\boldsymbol{x}_t + \beta_t \nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t)\right)$$

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

DDPM and Tweedie

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

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

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

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

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

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

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

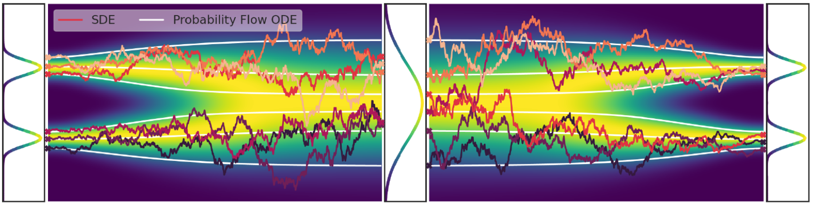
$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t, t)\right)$$

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

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

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)

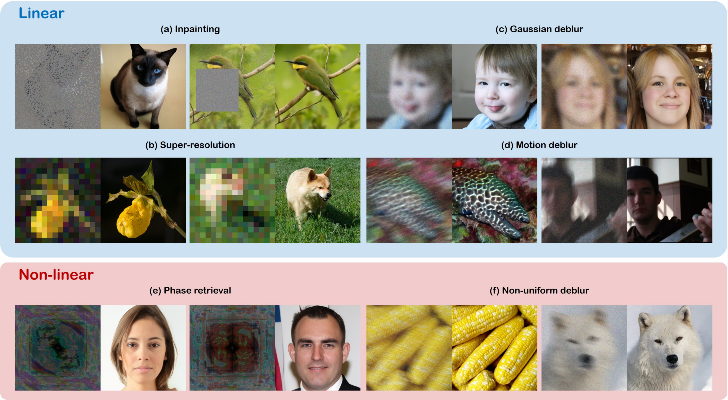


Figure 1: Solving noisy linear, and nonlinear inverse problems with diffusion models. Our reconstruction results (right) from the measurements (left) are shown.

(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.

Algorithm 1 DPS - Gaussian

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

1: $\boldsymbol{x}_N \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$
2: **for** $i = N-1$ **to** 0 **do**
3: $\quad \hat{\boldsymbol{s}} \leftarrow \boldsymbol{s}_\theta(\boldsymbol{x}_i, i)$
4: $\quad \hat{\boldsymbol{x}}_0 \leftarrow \frac{1}{\sqrt{\bar{\alpha}_i}}(\boldsymbol{x}_i + (1-\bar{\alpha}_i)\hat{\boldsymbol{s}})$
5: $\quad \boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$
6: $\quad \boldsymbol{x}'_{i-1} \leftarrow \frac{\sqrt{\alpha_i}(1-\bar{\alpha}_{i-1})}{1-\bar{\alpha}_i}\boldsymbol{x}_i + \frac{\sqrt{\bar{\alpha}_{i-1}}\beta_i}{1-\bar{\alpha}_i}\hat{\boldsymbol{x}}_0 + \tilde{\sigma}_i \boldsymbol{z}$
7: $\quad \boldsymbol{x}_{i-1} \leftarrow \boldsymbol{x}'_{i-1} - \zeta_i \nabla_{\boldsymbol{x}_i} \|\boldsymbol{y} - \mathcal{A}(\hat{\boldsymbol{x}}_0)\|_2^2$
8: **end for**
9: **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:

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

$t = 999$

Diffusion posterior sampling: Results

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

Inpainting:

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

$t = 900$

- 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:

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

$t = 700$

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

Inpainting:

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

$t = 600$

- 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:

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

$t = 200$

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

Inpainting:

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

$t = 100$

Diffusion posterior sampling: Results

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

Inpainting:

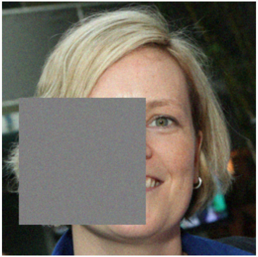
$\boldsymbol{x}_{\text{unknown}}$ $\boldsymbol{y}$ $\hat{\boldsymbol{x}}_0$ $\boldsymbol{x}_t$

$t = 0$

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 $\boldsymbol{x}_0$

- 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 $\boldsymbol{x}_0$

- 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))

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

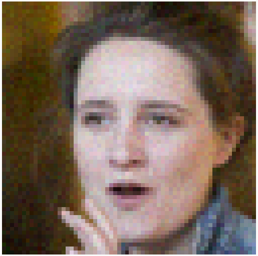
input $\boldsymbol{y}$

output $\boldsymbol{x}_0$

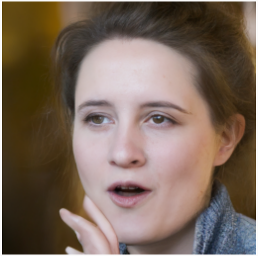
Diffusion posterior sampling: Super-resolution results

- 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 $\varepsilon_\theta(\boldsymbol{x}_t, \boldsymbol{y}_{\mathrm{LR}}, t)$.

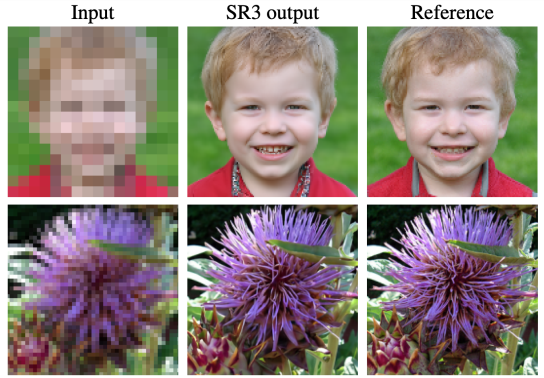


Figure 1: Two representative SR3 outputs: (top) $8\times$ face super-resolution at $16\times16\to128\times128$ pixels (bottom) $4\times$ natural image super-resolution at $64\times64\to256\times256$ pixels.

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."

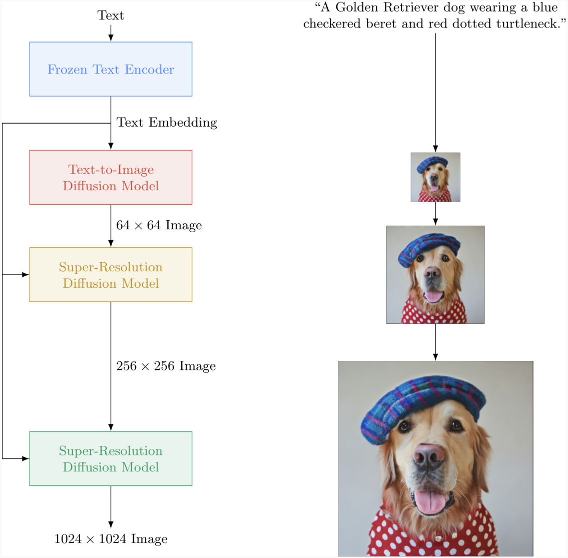
Conditional DDPM for super-resolution

Imagen pipeline:

Text conditioning

&

Conditional super-resolution via DDPM



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

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