Denoising Diffusion Probability Model

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Miao's Group - Paper Reading

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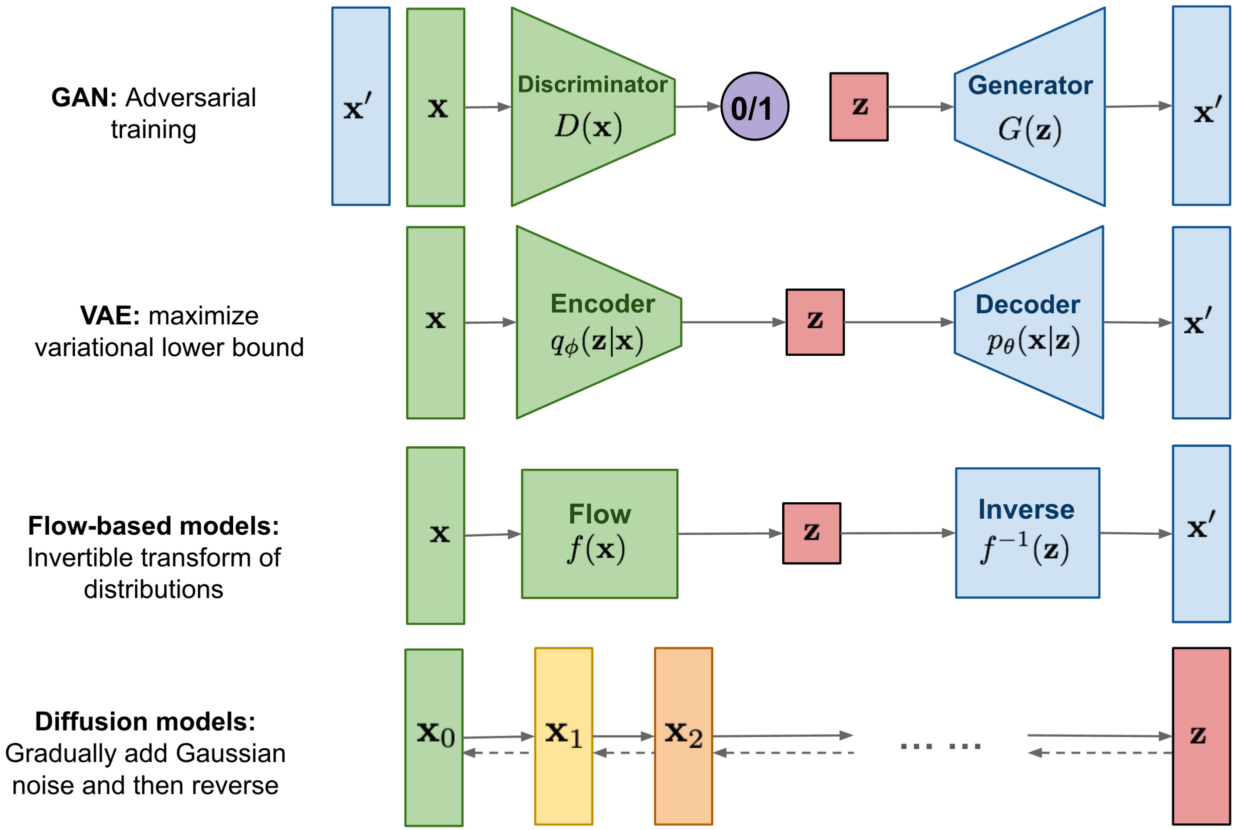
Image Generation Models



https://lilianweng.github.io/posts/2021-07-11-diffusion-models/#what-are-diffusion-models

Image Generation: GAN

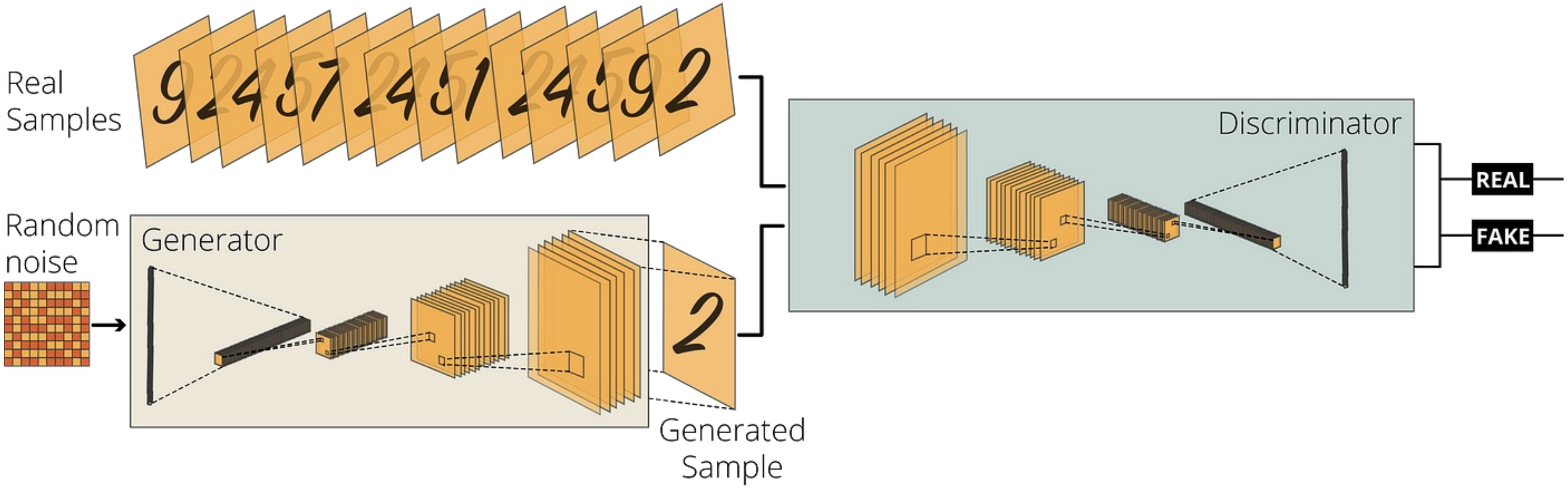
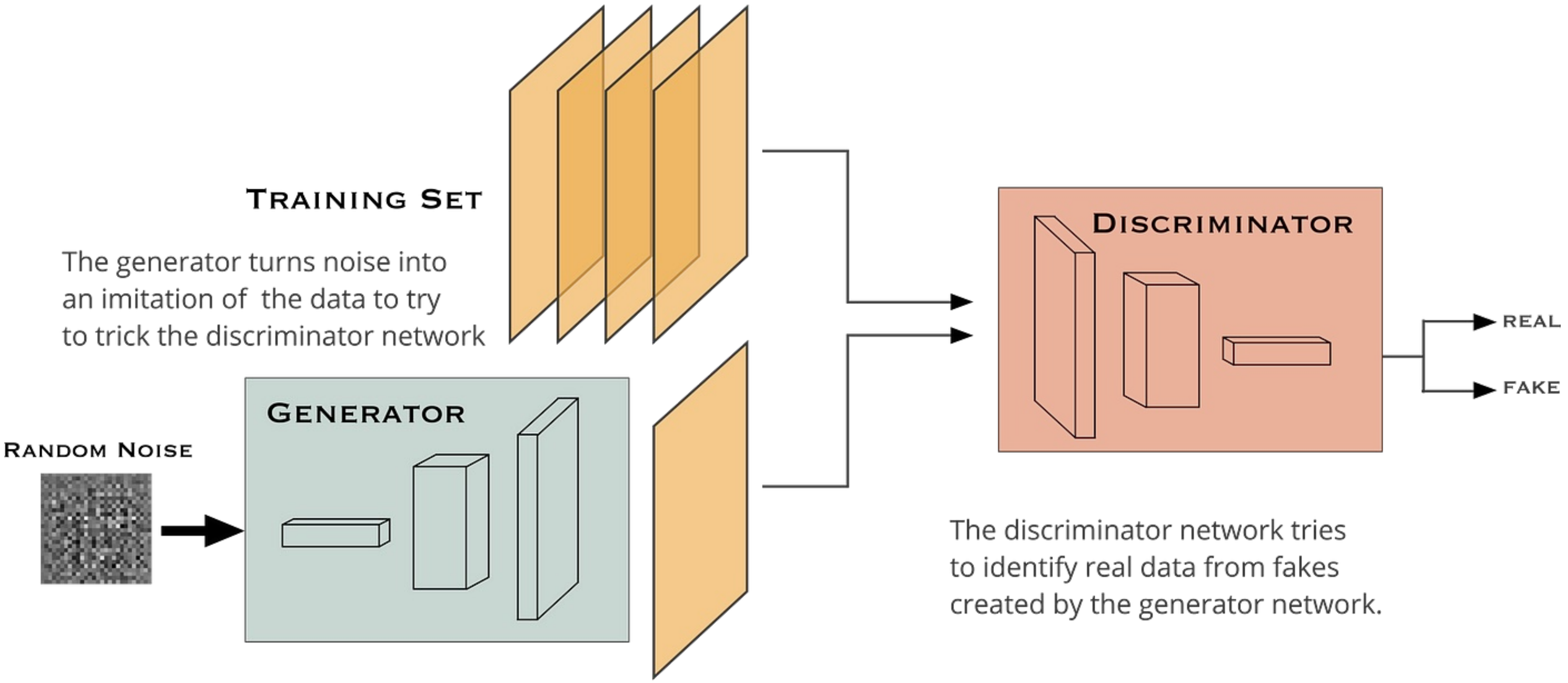


Figure adopted from: https://towardsdatascience.com/image-generation-in-10-minutes-with-generative-adversarial-networks-c2afc56bfa3b

Image Generation: GAN



https://towardsdatascience.com/image-generation-in-10-minutes-with-generative-adversarial-networks-c2afc56bfa3b

Image Generation: GAN

BigGAN: High-resolution image (train on 128x128 ImageNet images, generate 128/256/512 images

A. Brock, et al. “Large Scale GAN Training for High Fidelity Natural Image Synthesis,” ICLR, 2019.

Problems of GANs

- Difficult to train due to the adversarial nature of the problem formulation
- Outputs lack diversity
- Mode collapse
- Vanishing gradients
- Problem learning multimodal distribution

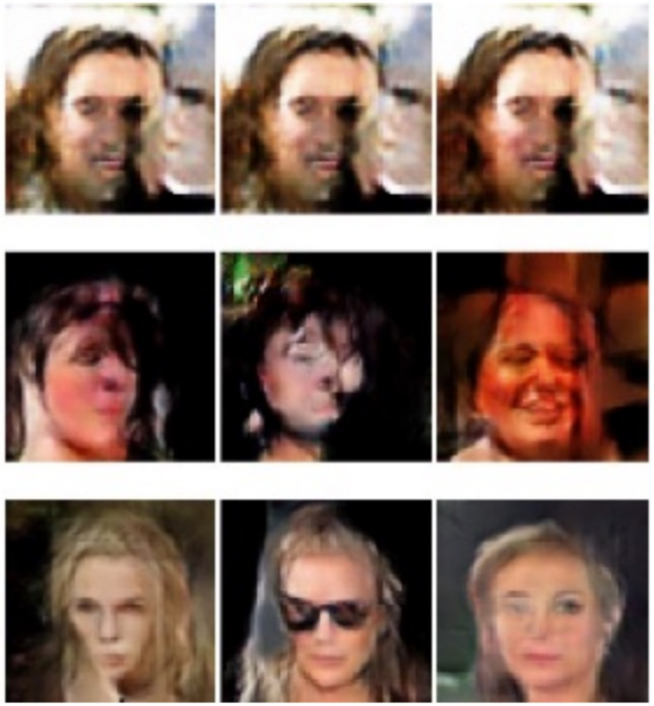
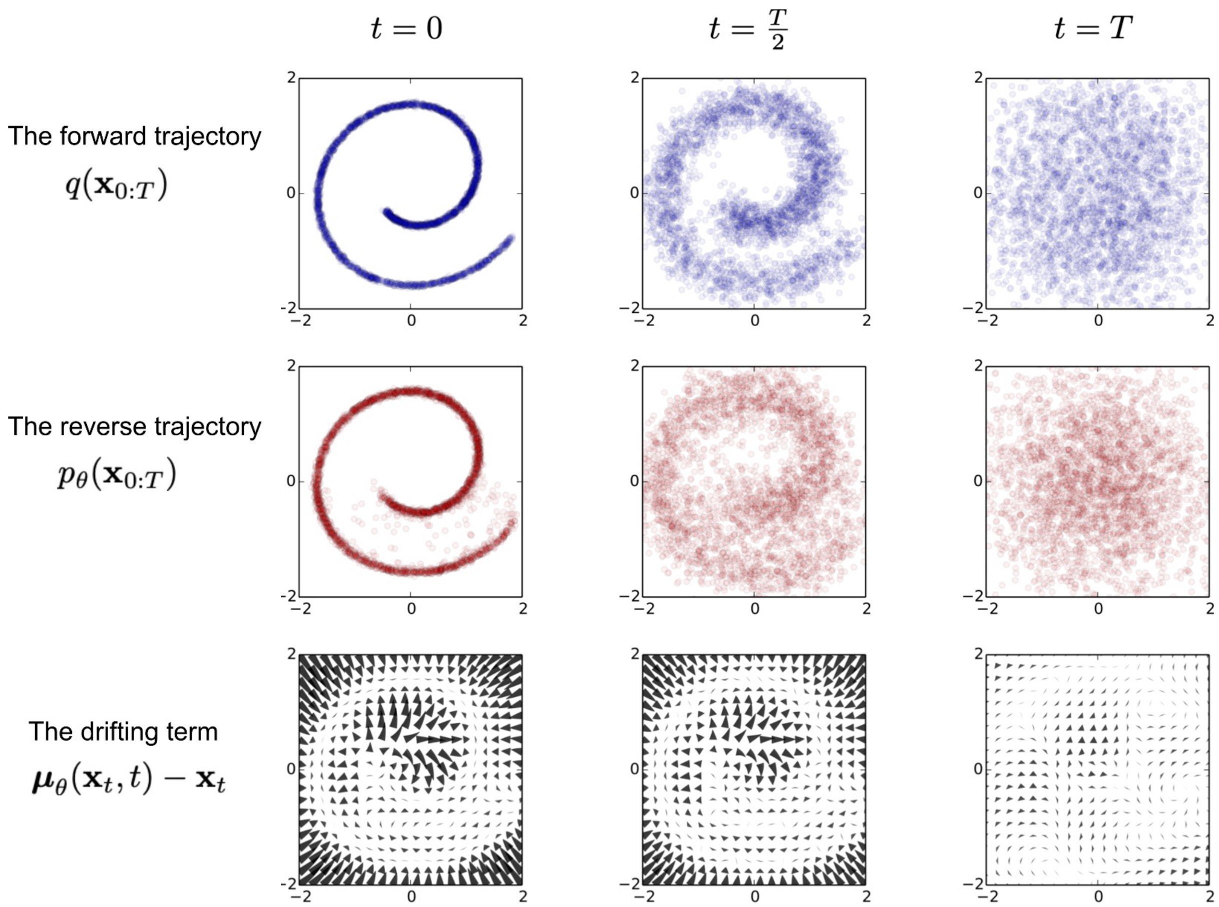


Image Generation: Diffusion Models

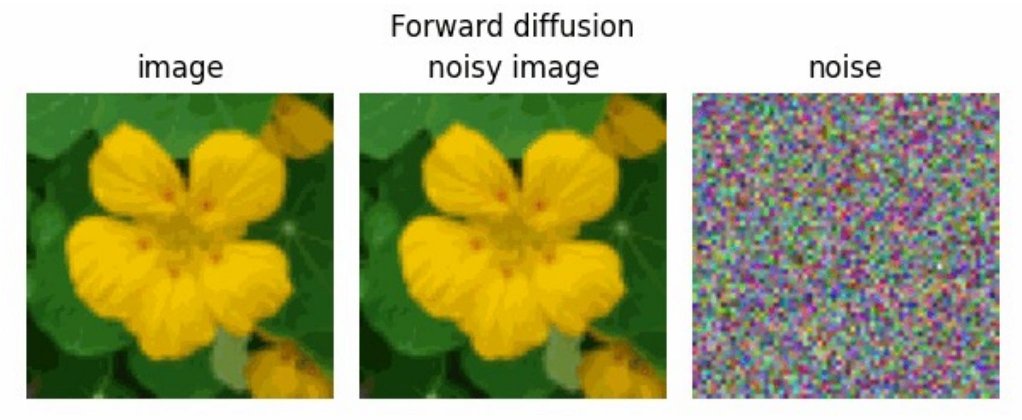
- The process originates from probabilistic likelihood estimation, and take inspiration from physical phenomenon
- Central idea comes from the thermodynamics of gas molecules, whereby the molecules diffuse from high density to low density areas
- This movement is often referred in physics literature as the increase of entropy



Sohl-Dickstein, et al. "Deep unsupervised learning using nonequilibrium thermodynamics." International conference on machine learning. PMLR, 2015.

Denoising Diffusion Probability Model

Statistical definition: *"Diffusion is the process of transforming a complex distribution into a predefined simpler one"*



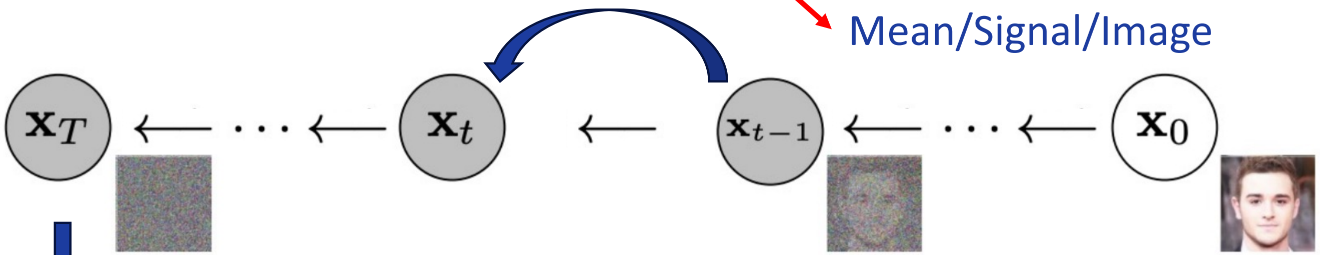
Denoising Diffusion Probability Model

Forward Diffusion Process

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

Variance

Mean/Signal/Image



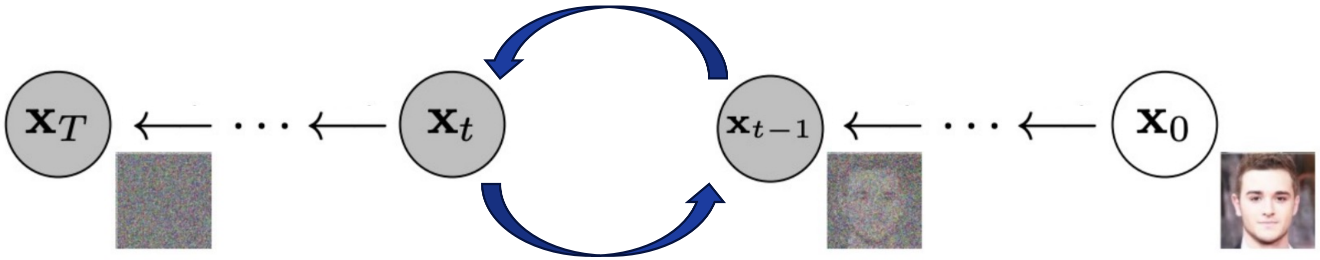
Markov process/ Markov chain

Isotropic Gaussian

Denoising Diffusion Probability Model

Reverse Diffusion Process

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

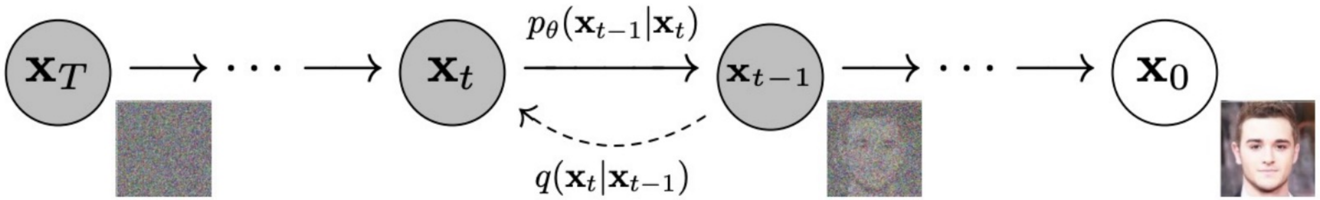


$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) \propto q(\mathbf{x}_{t-1})q(\mathbf{x}_t|\mathbf{x}_{t-1})$$ Intractable ➡ Machine Learning

Neural Network:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

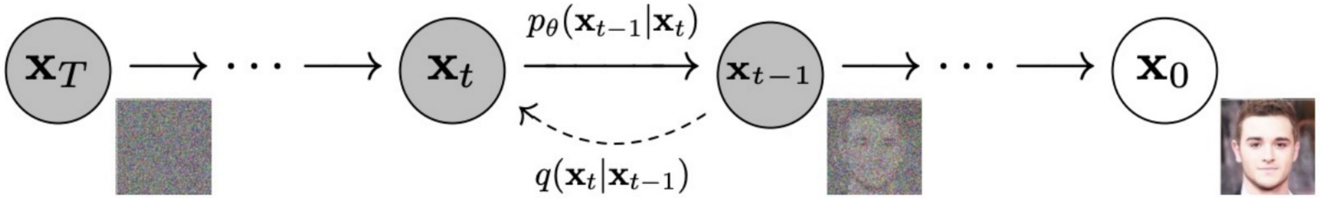
Denoising Diffusion Probability Model



Key concept behind:

- Denoising diffusion models; two steps: 1) forward, 2) reverse / reconstruction
- Build a learning model which can learn the systematic decay of information due to noise
- Reverse the process and therefore, recover the information back from the noise

Denoising Diffusion Probability Model



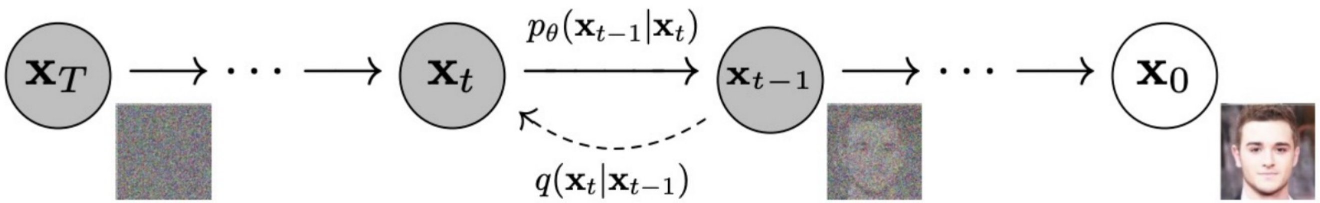
Forward diffusion:

- Gaussian noise is introduced successively until the data becomes all noise

Reverse diffusion:

- Undoes the noise by learning the conditional probability densities using a neural network

Denoising Diffusion Probability Model

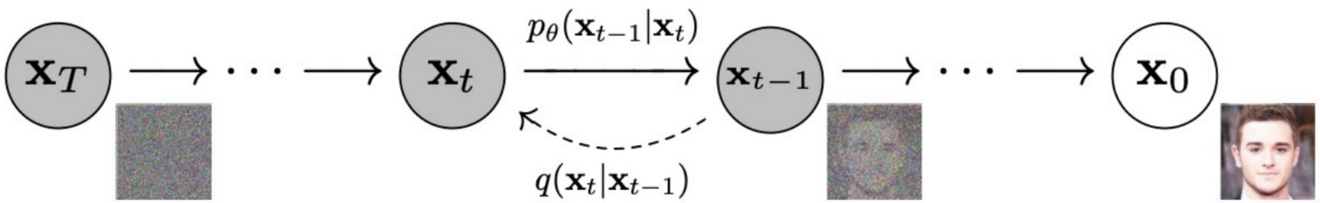


Forward step:

- We can formally define the forward diffusion process as a Markov Chain
- Starting with the initial data point, we add Gaussian noise for T successive steps, and obtain a set of noisy samples
- The prediction of probability density at time t is only dependent on the immediate predecessor at time $t - 1$
- The conditional probability density can be computed as:

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

Denoising Diffusion Probability Model



Forward step:

- The conditional probability density can be computed as:

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

- The complete distribution of the whole process can then be computed as follows:

$$q(\mathbf{x}_{0:T}|\mathbf{x}_0) = q(\mathbf{x}_0)\prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

- The mean and variance of the density function depends on a parameter β_t, which is a hyper parameter whose value can either be taken as a constant throughout the process or can be gradually changed in the successive steps

Denoising Diffusion Probability Model

Forward step:

- The above derivation is enough to predict the successive states
- We would like to sample at any given time interval t without going through all the intermediary steps
- This allows an efficient implementation
- Re-formulation:

$$\alpha_t = 1 - \beta_t, \bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} \\ &= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\boldsymbol{\epsilon}}_{t-2} \\ &= \cdots \\ &= \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}\end{aligned}$$

Conditional probability density:

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

Complete distribution:

$$q(\mathbf{x}_{0:T}|\mathbf{x}_0) = q(\mathbf{x}_0)\prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

$$\Longrightarrow \quad q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\boldsymbol{I})$$

Denoising Diffusion Probability Model

Reverse step:

- The reverse process requires the estimation of probability density at an earlier time step given the current state of the system
- This means estimating the $q(\mathbf{x}_t|\mathbf{x}_{t-1})$ when $t = T$
- Thereby generating data sample from isotropic Gaussian noise
- The estimation of previous state from the current state requires the knowledge of all the previous gradients which we can't obtain without having a learning model that can predict such estimates

Conditional probability density:

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

Complete distribution:

$$q(\mathbf{x}_{0:T}|\mathbf{x}_0) = q(\mathbf{x}_0)\prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

Re-formulation:

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\boldsymbol{I})$$

Denoising Diffusion Probability Model

Reverse step:

- The estimation of previous state from the current state requires the knowledge of all the previous gradients which we can't obtain without having a learning model that can predict such estimates
- Solution
  - Train a neural network that estimates the $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ based on learned weights θ and the current state at time t
  - Formulated as:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_t) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

Conditional probability density:

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

Complete distribution:

$$q(\mathbf{x}_{0:T}|\mathbf{x}_0) = q(\mathbf{x}_0) \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

Re-formulation:

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\boldsymbol{I})$$

Denoising Diffusion Probability Model

Reverse step:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \Rightarrow q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \boldsymbol{I})$$

$$\begin{aligned}
&q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \\
&\quad = q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} \\
&\quad \propto \exp\left(-\frac{1}{2}\left(\frac{\left(\mathbf{x}_t - \sqrt{\alpha_t}\mathbf{x}_{t-1}\right)^2}{\beta_t} + \frac{\left(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0\right)^2}{1-\bar{\alpha}_{t-1}} - \frac{\left(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0\right)^2}{1-\bar{\alpha}_t}\right)\right) \\
&\quad = \exp\left(-\frac{1}{2}\left(\frac{\mathbf{x}_t^2 - 2\sqrt{\alpha_t}\mathbf{x}_t\mathbf{x}_{t-1} + \alpha_t\mathbf{x}_{t-1}^2}{\beta_t} + \frac{\mathbf{x}_{t-1}^2 - 2\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0\mathbf{x}_{t-1} + \bar{\alpha}_{t-1}\mathbf{x}_0^2}{1-\bar{\alpha}_{t-1}} - \frac{\left(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0\right)^2}{1-\bar{\alpha}_t}\right)\right) \\
&\quad = \exp\left(-\frac{1}{2}\left(\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\right)\mathbf{x}_{t-1}^2 - \left(\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0\right)\mathbf{x}_{t-1} + C(\mathbf{x}_t, \mathbf{x}_0)\right)\right)
\end{aligned}$$

Denoising Diffusion Probability Model

$$\alpha_t = 1 - \beta_t, \bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

Reverse step:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \Rightarrow q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \boldsymbol{I})$$

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \exp\left(-\frac{1}{2}\left(\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\right)\mathbf{x}_{t-1}^2 - \left(\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0\right)\mathbf{x}_{t-1} + C(\mathbf{x}_t, \mathbf{x}_0)\right)\right)$$

$$\tilde{\beta}_t = 1/\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\right) = 1/\left(\frac{\alpha_t - \bar{\alpha}_t + \beta_t}{\beta_t(1-\bar{\alpha}_{t-1})}\right) = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t$$

$$\tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0) = \left(\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0\right) / \left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\right)$$

$$= \left(\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0\right)\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t$$

$$= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t$$

$$\mathbf{x}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\left(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t\right)$$

Denoising Diffusion Probability Model

Reverse step:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \Rightarrow q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \boldsymbol{I})$$

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

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

Denoising Diffusion Probability Model

Reverse step:

- The parameterization for:
  - Mean function:

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

  - Variance function (fixed as $\boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t) = \sigma_t^2 \boldsymbol{I}$, $\sigma_t^2 = \beta_t$ or $\sigma_t^2 = \tilde{\beta}_t$):

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$$

Current state estimation:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

Denoising Diffusion Probability Model

Loss:

$$
\begin{aligned}
-\log p_\theta &\leq -\log p_\theta(\mathbf{x}_0) + D_{KL}\left((q(\mathbf{x}_{1:T}|\mathbf{x}_0)||p_\theta(\mathbf{x}_{1:T}|\mathbf{x}_0))\right) \\
&= -\log p_\theta(\mathbf{x}_0) + \mathbb{E}_{\mathbf{x}_{1:T}\sim q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})/p_\theta(\mathbf{x}_0)}\right] \\
&= -\log p_\theta(\mathbf{x}_0) + \mathbb{E}_q\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})} + \log p_\theta(\mathbf{x}_0)\right] \\
&= \mathbb{E}_q\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\right] \\
&= L_{VLB}
\end{aligned}
$$

Denoising Diffusion Probability Model

Loss:

$$
\begin{aligned}
L_{VLB} &= \mathbb{E}_{q(\mathbf{x}_{0:T})}\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\right] \\
&= \mathbb{E}_q\left[\log \frac{\Pi_{t=t}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_T)\Pi_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}\right] \\
&= \mathbb{E}_q\left[-\log p_\theta(\mathbf{x}_T) + \sum_{t=1}^{T} \log \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}\right] \\
&= \mathbb{E}_q\left[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} + \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\right] \\
&= \mathbb{E}_q\left[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T} \log \left(\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} \cdot \frac{q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}\right) + \log \frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\right]
\end{aligned}
$$

Denoising Diffusion Probability Model

Loss:

$$
\begin{aligned}
L_{VLB} &= \mathbb{E}_q\left[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T} \log\left(\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} \cdot \frac{q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}\right) + \log\frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\right] \\
&= \mathbb{E}_q\left[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T} \log\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} + \sum_{t=2}^{T} \log\frac{q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)} + \log\frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\right] \\
&= \mathbb{E}_q\left[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^{T} \log\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} + \log\frac{q(\mathbf{x}_T|\mathbf{x}_0)}{q(\mathbf{x}_1|\mathbf{x}_0)} + \log\frac{q(\mathbf{x}_1|\mathbf{x}_0)}{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}\right] \\
&= \mathbb{E}_q\left[\log\frac{q(\mathbf{x}_T|\mathbf{x}_0)}{p_\theta(\mathbf{x}_T)} + \sum_{t=2}^{T} \log\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)} - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)\right] \\
&= \mathbb{E}_q\left[\mathrm{D}_{KL}\left(q(\mathbf{x}_T|\mathbf{x}_0)||p_\theta(\mathbf{x}_T)\right) + \sum_{t=2}^{T} D_{KL}\left(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)\right) - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)\right]
\end{aligned}
$$

Denoising Diffusion Probability Model

Loss:

$$L_{VLB} = \mathbb{E}_q\left[\underbrace{D_{KL}\left(q(\mathbf{x}_T|\mathbf{x}_0)||p_\theta(\mathbf{x}_T)\right)}_{L_T} + \sum_{t=2}^{T}\underbrace{D_{KL}\left(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)\right)}_{L_t}\underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\right]$$

$$L_{VLB} = L_T + L_{T-1} + \cdots + L_0$$

Denoising Diffusion Probability Model

Loss:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \Rightarrow q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \boldsymbol{I})$$

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

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

$$L_t = D_{KL}\left(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)\right) = \mathbb{E}_{\mathbf{x}_0, \epsilon}\frac{1}{2\|\boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)\|^2}\|\tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, \mathrm{t})\|$$

$$L_t^{simple} = \mathbb{E}_{t\sim[1,T]\mathbf{x}_0, \boldsymbol{\epsilon}}\|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, \mathrm{t})\| = \mathbb{E}_{t\sim[1,T]\mathbf{x}_0, \boldsymbol{\epsilon}}\|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, \mathrm{t})\|$$

Denoising Diffusion Probability Model

Algorithm:

Algorithm 1 Training

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

Denoising Diffusion Probability Model

Generation Ability:

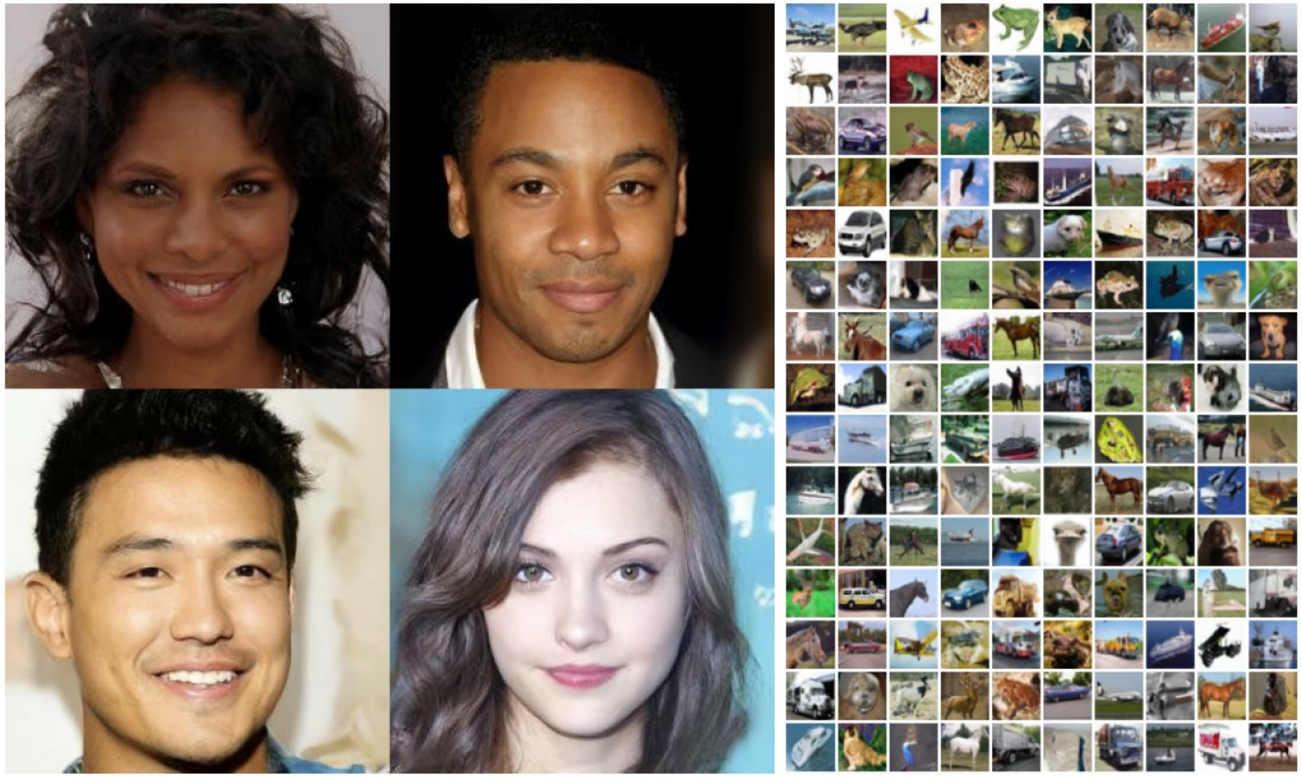


Figure 1: Generated samples on CelebA-HQ 256 × 256 (left) and unconditional CIFAR10 (right)

Denoising Diffusion Probability Model

Generation Ability:

Table 1: CIFAR10 results. NLL measured in bits/dim.

Model	IS	FID	NLL Test (Train)
Conditional			
EBM [11]	8.30	37.9	
JEM [17]	8.76	38.4	
BigGAN [3]	9.22	14.73	
StyleGAN2 + ADA (v1) [29]	**10.06**	**2.67**	
Unconditional			
Diffusion (original) [53]			≤ 5.40
Gated PixelCNN [59]	4.60	65.93	3.03 (2.90)
Sparse Transformer [7]			**2.80**
PixelIQN [43]	5.29	49.46	
EBM [11]	6.78	38.2	
NCSNv2 [56]		31.75	
NCSN [55]	8.87±0.12	25.32	
SNGAN [39]	8.22±0.05	21.7	
SNGAN-DDLS [4]	9.09±0.10	15.42	
StyleGAN2 + ADA (v1) [29]	**9.74** ± 0.05	3.26	
Ours (L, fixed isotropic $\mathbf{\Sigma}$)	7.67±0.13	13.51	≤ 3.70 (3.69)
Ours (L_{simple})	9.46±0.11	**3.17**	≤ 3.75 (3.72)

Denoising Diffusion Probability Model

Beat GAN:

Model	FID	sFID	Prec	Rec
LSUN Bedrooms 256×256				
DCTransformer† [42]	6.40	6.66	0.44	**0.56**
DDPM [25]	4.89	9.07	0.60	0.45
IDDPM [43]	4.24	8.21	0.62	0.46
StyleGAN [27]	2.35	6.62	0.59	0.48
ADM (dropout)	**1.90**	**5.59**	**0.66**	0.51
LSUN Horses 256×256				
StyleGAN2 [28]	3.84	6.46	0.63	0.48
ADM	2.95	**5.94**	0.69	**0.55**
ADM (dropout)	**2.57**	6.81	**0.71**	**0.55**
LSUN Cats 256×256				
DDPM [25]	17.1	12.4	0.53	0.48
StyleGAN2 [28]	7.25	**6.33**	0.58	0.43
ADM (dropout)	**5.57**	6.69	**0.63**	**0.52**
ImageNet 64×64				
BigGAN-deep* [5]	4.06	3.96	**0.79**	0.48
IDDPM [43]	2.92	**3.79**	0.74	0.62
ADM	2.61	**3.77**	0.73	0.63
ADM (dropout)	**2.07**	4.29	0.74	**0.63**

Model	FID	sFID	Prec	Rec
ImageNet 128×128				
BigGAN-deep [5]	6.02	7.18	**0.86**	0.35
LOGAN† [68]	3.36			
ADM	5.91	**5.09**	0.70	**0.65**
ADM-G (25 steps)	5.98	7.04	0.78	0.51
ADM-G	**2.97**	**5.09**	0.78	0.59
ImageNet 256×256				
DCTransformer† [42]	36.51	8.24	0.36	**0.67**
VQ-VAE-2†‡ [51]	31.11	17.38	0.36	0.57
IDDPM‡ [43]	12.26	5.42	0.70	0.62
SR3†‡ [53]	11.30			
BigGAN-deep [5]	6.95	7.36	**0.87**	0.28
ADM	10.94	6.02	0.69	0.63
ADM-G (25 steps)	5.44	5.32	0.81	0.49
ADM-G	**4.59**	**5.25**	0.82	0.52
ImageNet 512×512				
BigGAN-deep [5]	8.43	8.13	**0.88**	0.29
ADM	23.24	10.19	0.73	**0.60**
ADM-G (25 steps)	8.41	9.67	0.83	0.47
ADM-G	**7.72**	**6.57**	0.87	0.42

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Q&A

Thanks

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Miao’s Group - Paper Reading

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