Denoising Diffusion Probabilistic Model

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Artificial Intelligence

Creating the Future

Dong-A University

Division of Computer Engineering &
Artificial Intelligence

References

Jonathan Ho, Ajay Jain, Pieter Abbeel, "Denoising Diffusion Probabilistic Model," NeurIPS 2020
UC Berkeley

https://github.com/hojonathanho/diffusion
https://hojonathanho.github.io/diffusion/

[Blog]
https://happy-jihye.github.io/diffusion/diffusion-1/

[DPM]
https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

[DDPM]
PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc
http://dsba.korea.ac.kr/seminar/?mod=document&uid=2352

Denoising Diffusion Probabilistic Models (DDPM)

Jonathan Ho, Ajay Jain, Pieter Abbeel
NeurIPS 2020
UC Berkeley
https://github.com/hojonathanho/diffusion
https://hojonathanho.github.io/diffusion/

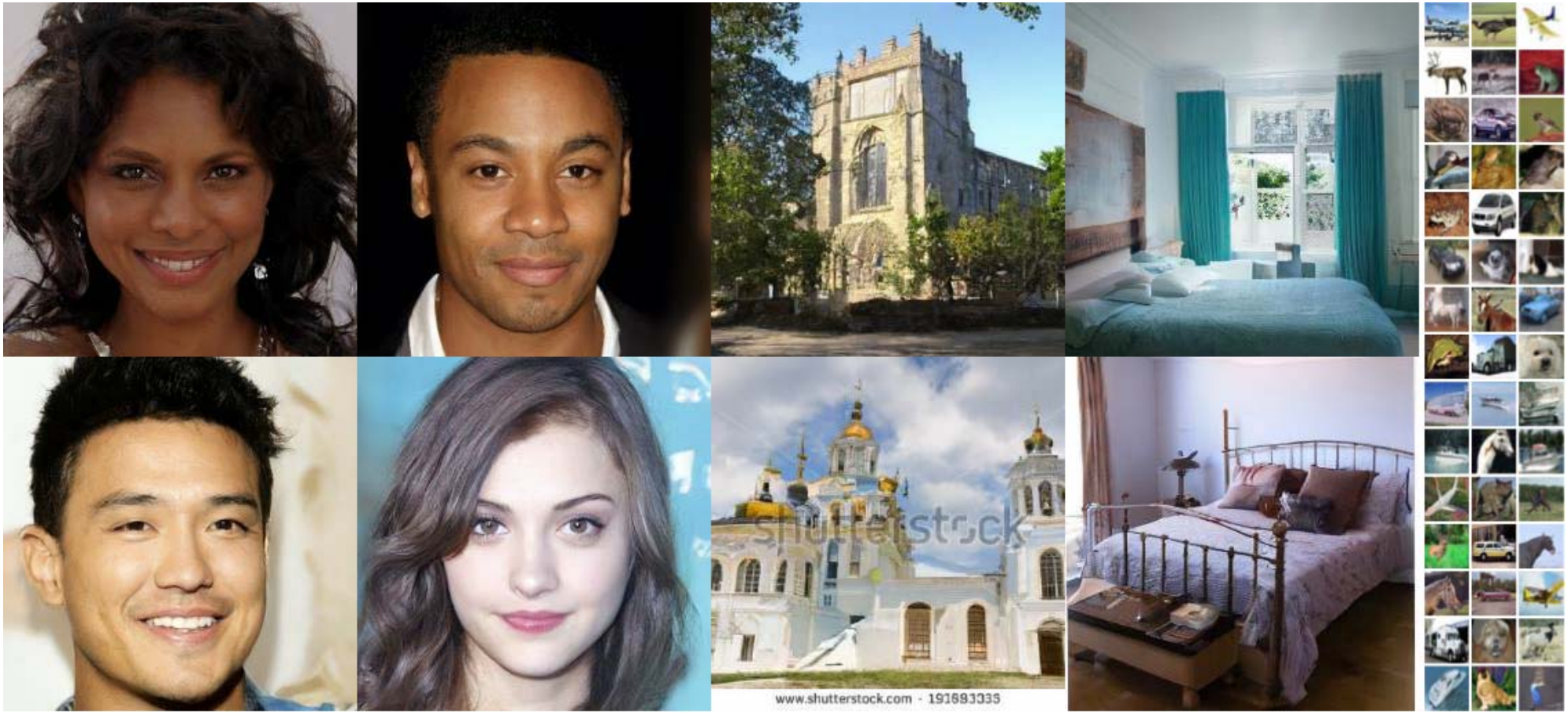
PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc

Abstract

- We present high quality image synthesis results using **diffusion probabilistic models**, a class of latent variable models inspired by considerations from **nonequilibrium thermodynamics**.
- Our best results are obtained by **training on a weighted variational bound** designed according to a novel connection **between diffusion probabilistic models and denoising score matching with Langevin dynamics**, and our models naturally admit a **progressive lossy decompression scheme** that can be interpreted as **a generalization of autoregressive decoding**. On the unconditional CIFAR10 dataset, we obtain an Inception score of 9.46 and a state-of-the-art FID score of 3.17. On 256x256 LSUN, we obtain sample quality similar to ProgressiveGAN.

Denoising Diffusion Probabilistic Models (DDPM)

PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc



Denoising Diffusion Probabilistic Models (DDPM)

Generative Models

PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc

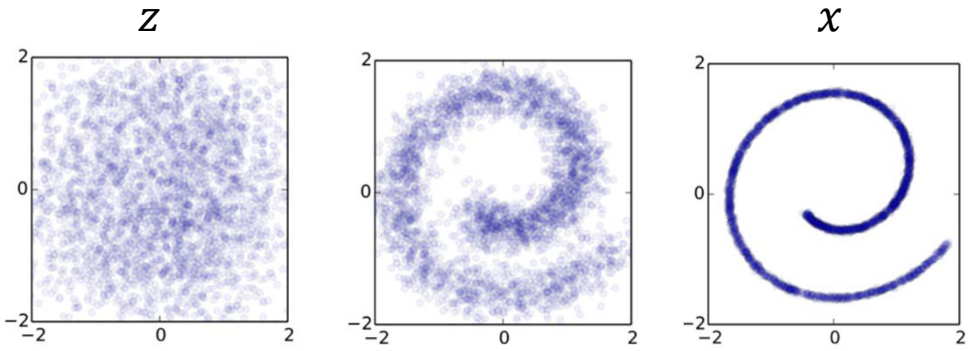
“To know the distribution(manifold) of data”

Variational Autoencoders

GANs

Normalizing Flow

https://www.youtube.com/watch?v=TywKpiZJ7P4



High Entropy
Low Information

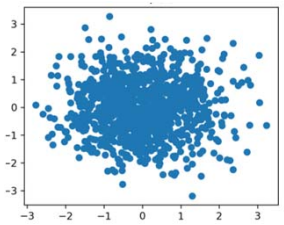
Low Entropy
High Information

Generative Models

http://dsba.korea.ac.kr/seminar/?mod=document&uid=2352

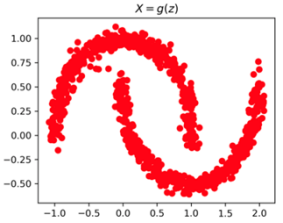
Generative Model : Latent variable model

$p_z(z) \sim N$



Trained model

$p'_x(x)$



✓ *Simple distribution*

✓ *Tractable(Gaussian)*

Input

✓ *Complex distribution*

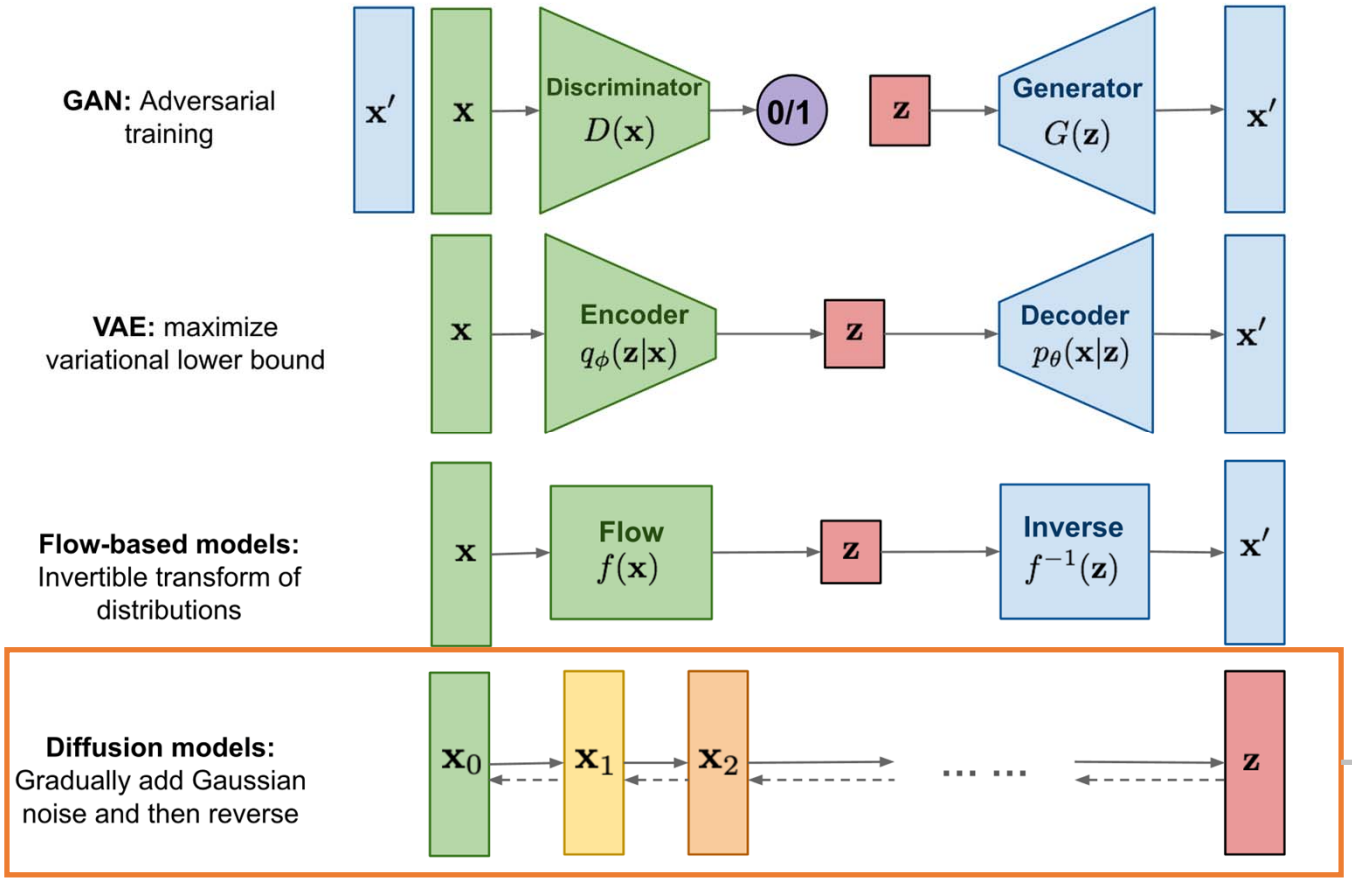
✓ *Visual, Audio patterns*

Output

- 결국 생성 모델로부터 **원하는 것은 매우 간단한 분포(Z)를 특정한 패턴을 갖는 분포로 변환**(mapping, transformation, sampling)하는 것
- 그렇기에 **대부분의 생성모델**이 주어진 입력 데이터로부터 **latent variable(Z)**을 얻어내고, 이를 **변환하는 역량을 학습**하고자 함

Denoising Diffusion Probabilistic Models (DDPM)

Generative Models



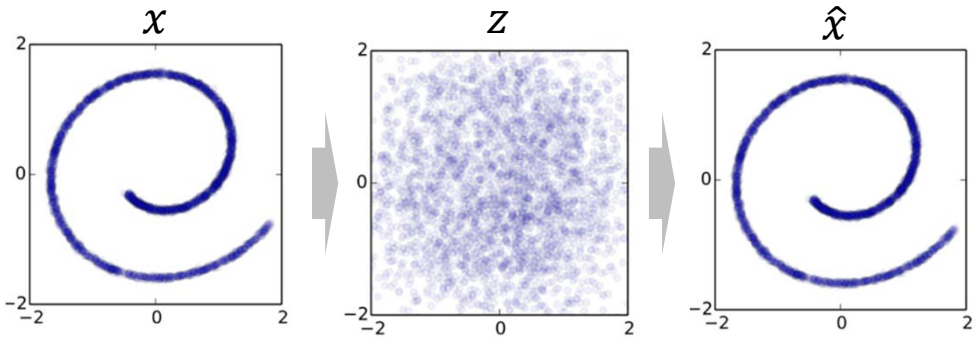
- 반복적인 변화(**iterative transformation**)를 활용한다는 점에서 **Flow-based models** 와 유사
- 분포에 대한 **Variational Inference**을 통한 학습을 진행한다는 점은 **VAE**와 유사
- 최근에는 Diffusion 모델의 학습에 Adversarial training을 활용하기도 함 (Diffusion-GAN, 2022)

Denoising Diffusion Probabilistic Models (DDPM)

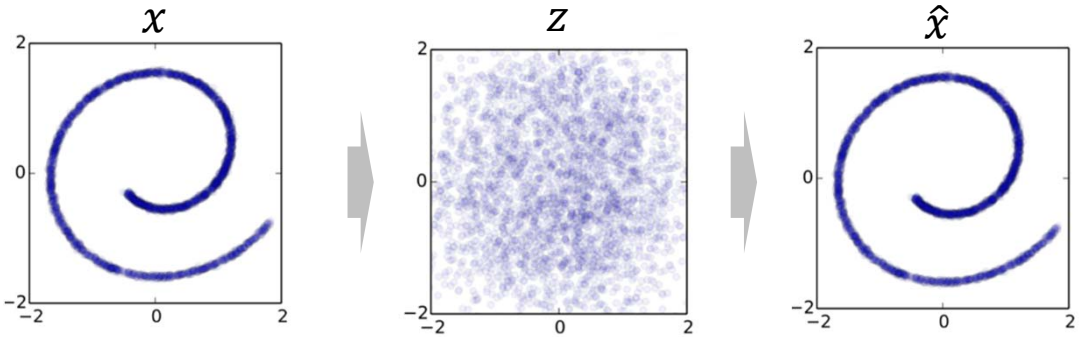
Generative Models

PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc

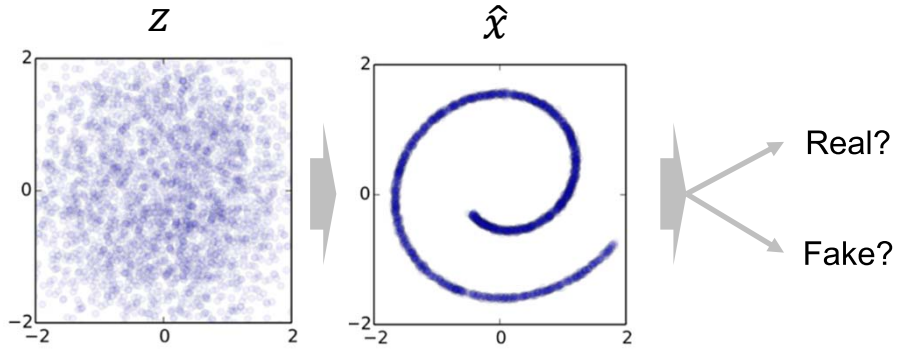
Variational Autoencoders



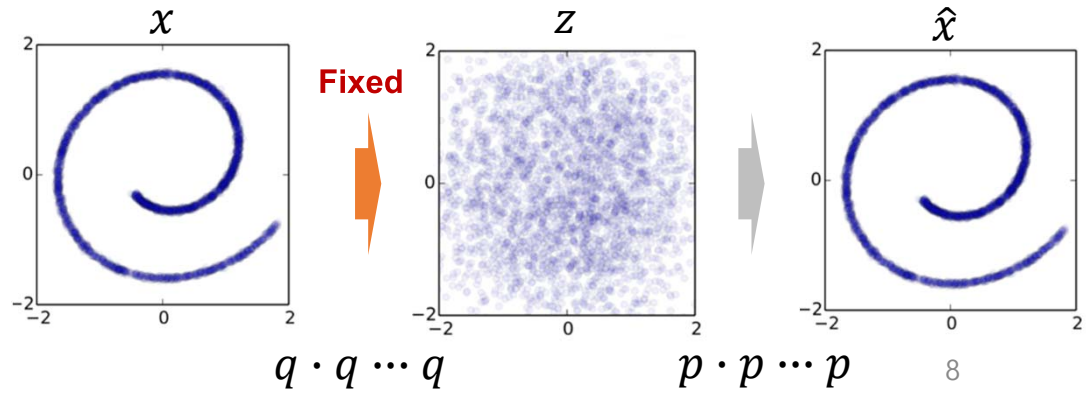
Normalizing Flow



GANs

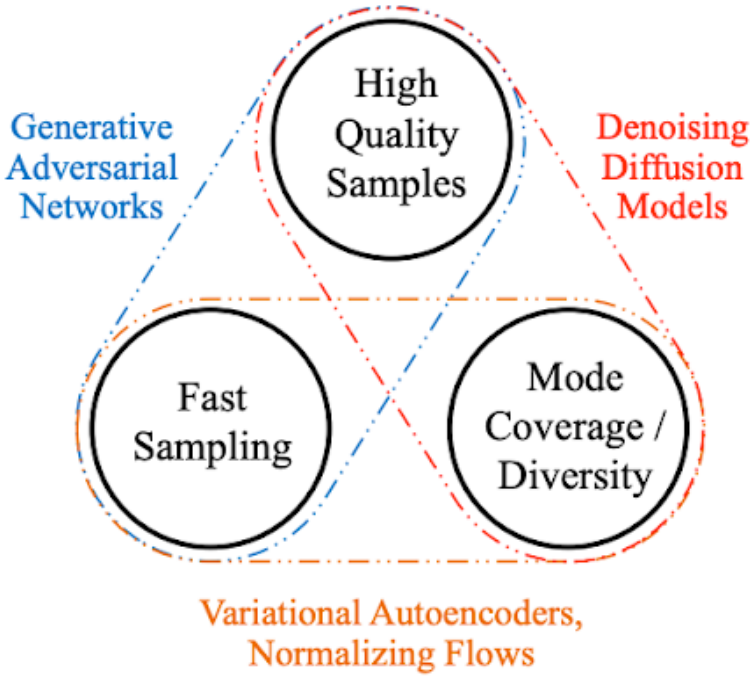


Diffusion Model



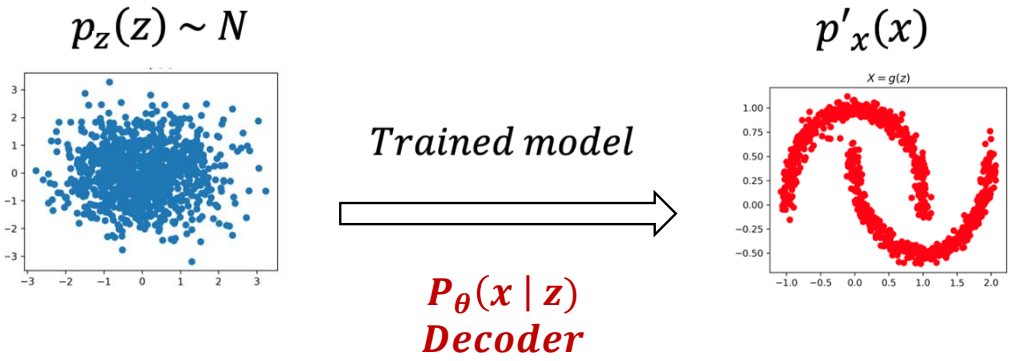
Denoising Diffusion Probabilistic Models (DDPM)

Generative Models



Generative Models

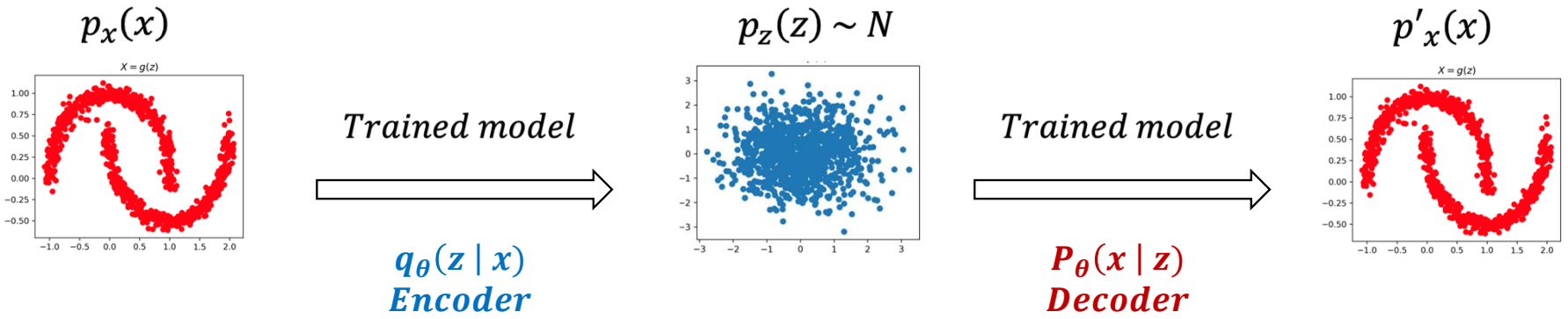
Variational Autoencoders



- 학습된 **Decoder network**를 통해 latent variable을 특정한 패턴의 분포로 mapping

Generative Models

Variational Autoencoders

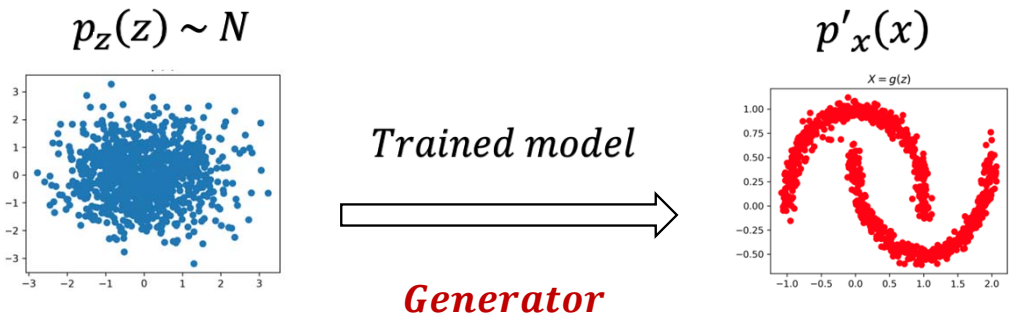


- **Encoder**를 모델 구조에 추가해, **Latent variable** / **Encoder** / **Decoder**를 모두 학습

$$P_\theta(x) = \frac{P_\theta(x|z)\boldsymbol{P_\theta(z)}}{P_\theta(z|x)} = likelihood$$

Generative Models

GAN



- 학습된 **Generator**를 통해 latent variable을 특정한 패턴의 분포로 mapping

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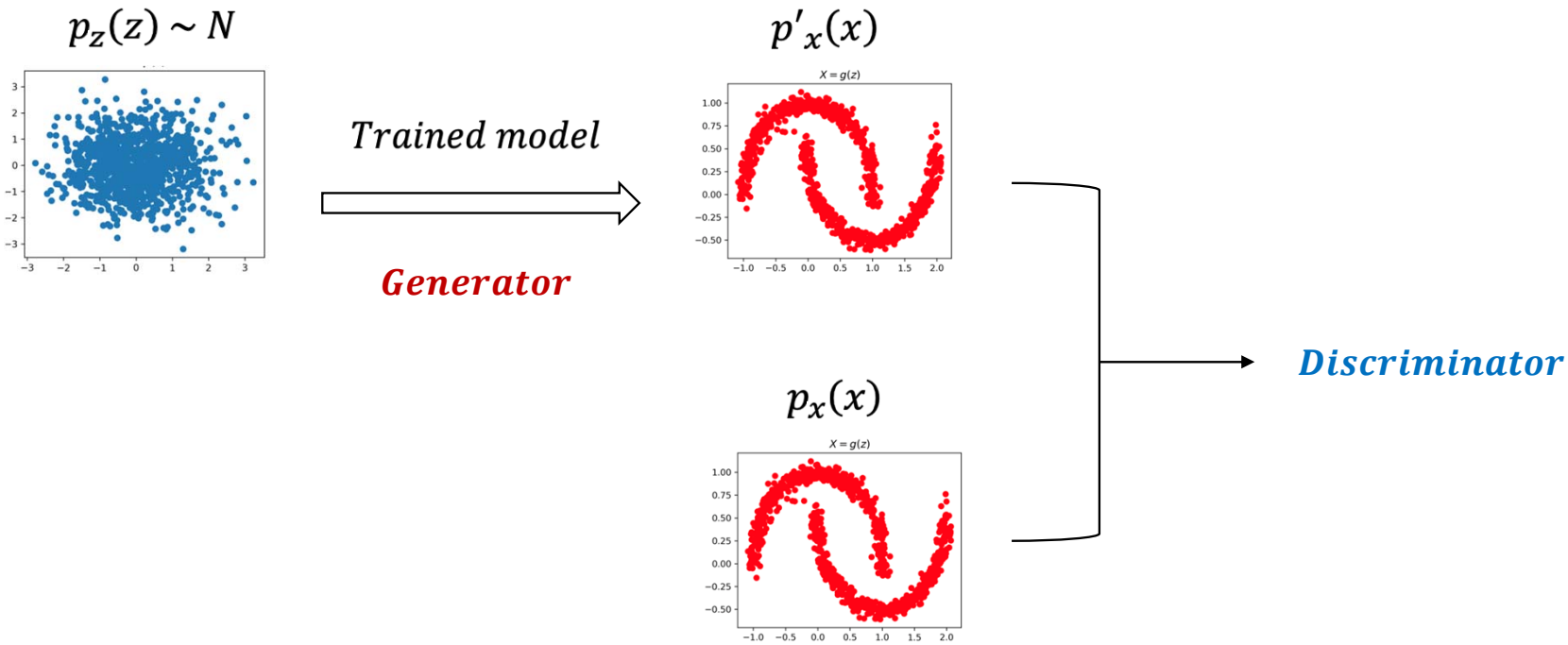
Generative Models

GAN

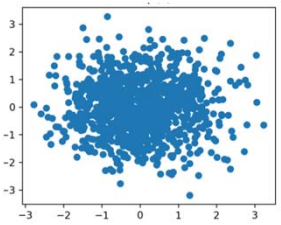


- **Discriminator**를 모델 구조에 추가해, **Generator**를 학습

Generative Models

Flow-based Model

$p_z(z) \sim N$



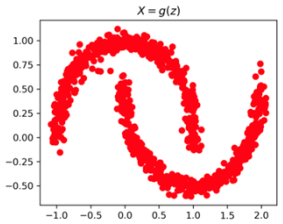
$Trained\ model$

$f^{-1} \circ f^{-1} \circ \ldots \circ f^{-1}$

$Flow\ (inverse)$

$(Chain\ of\ functions)$

$p'_x(x)$

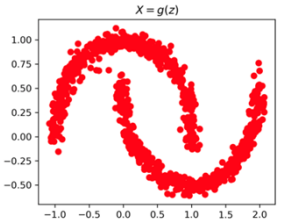


- 학습된 **Flow model**의 **Inverse mapping**을 통해 latent variable을 특정한 패턴의 분포로 mapping

Generative Models

Flow-based Model

$p_x(x)$



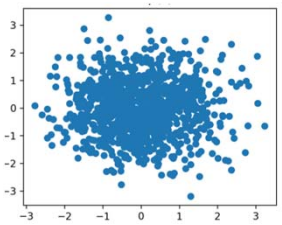
Trained model

$f \circ f \circ \ldots \circ f$

$\boldsymbol{Flow\ (forward)}$

$\boldsymbol{(Chain\ of\ functions)}$

$p_z(z) \sim N$



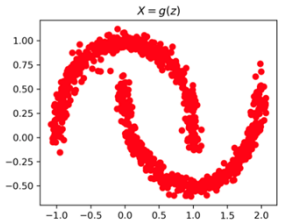
Trained model

$f^{-1} \circ f^{-1} \circ \ldots \circ f^{-1}$

$\boldsymbol{Flow\ (inverse)}$

$\boldsymbol{(Chain\ of\ functions)}$

$p'_x(x)$



- 생성에 활용되는 **Inverse mapping**을 학습하기 위해 **Invertible function**을 학습

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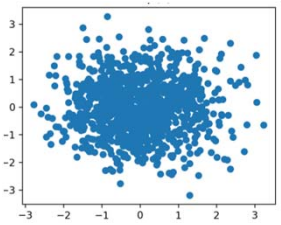
Generative Models

Diffusion based generative model

$p_z(z) \sim N$

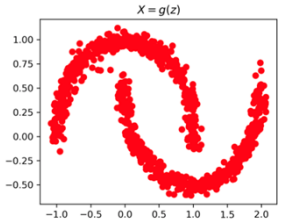


Trained model

$P_\theta(x \mid z)$

Sampling process

$p'_x(x)$



- 학습된 **Diffusion model**의 조건부 확률 분포 $P_\theta(x \mid z)$ 를 통해 특정한 패턴의 분포 획득

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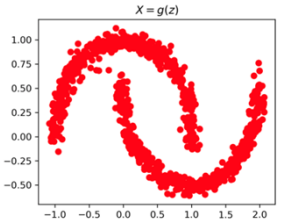
Generative Models

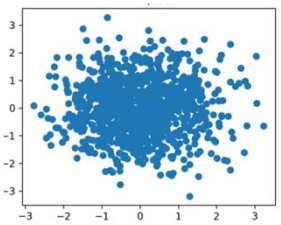
Diffusion based generative model

$p_x(x)$



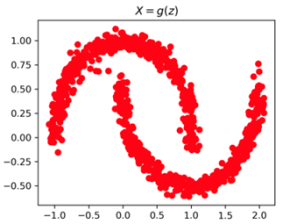
Fixed noise schedule

$p_z(z) \sim N$



Trained model

$p'_x(x)$



Iterative Markov chain

$$q(x_1|x_0) \circ q(x_2|x_1) \circ \cdots \circ q(x_T = z|x_{T-1})$$

$$q(z \mid x)$$

Diffusion process

Iterative Markov chain

$$P_\theta(z_1|z_0) \circ P_\theta(z_2|z_1) \circ \cdots \circ P_\theta(z_T = x|z_{T-1})$$

$$P_\theta(x \mid z)$$

Sampling process

- 생성에 활용되는 조건부 확률 분포 $P_\theta(x \mid z)$ 을 학습하기 위해 **Diffusion process** $q(z \mid x)$ 를 활용

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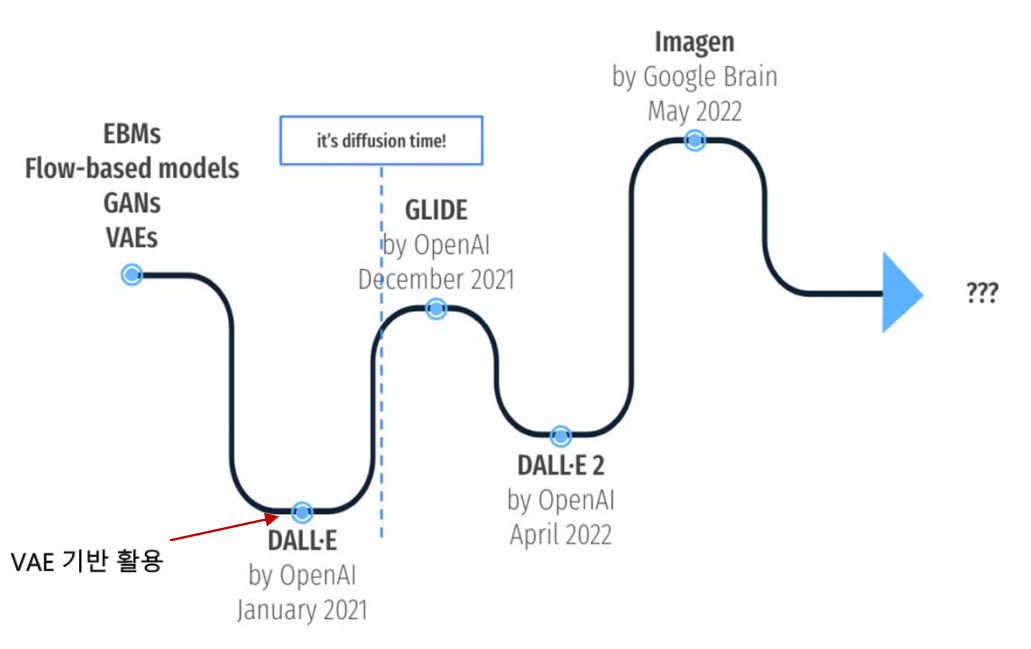
Diffusion Model Overview

➢ Diffusion Model 활용 : Text-to-Image generation



"An astronaut riding a horse in a photorealistic style"

↓

DALLE 2

↓

"A brain riding a rocketship heading towards the moon"

↓

Imagen

↓

- 2021년부터 Diffusion based generative model을 활용한 다양한 Text-to-Image generation 방법론이 제안되며 눈길을 끔
- 이미지, 오디오 등 다양한 양식의 벤치마크 데이터에서 리더보드 상위권에 오르며 generation 성능을 확인함

Denoising Diffusion Probabilistic Models (DDPM)

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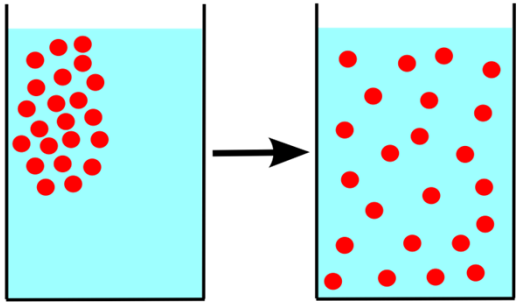
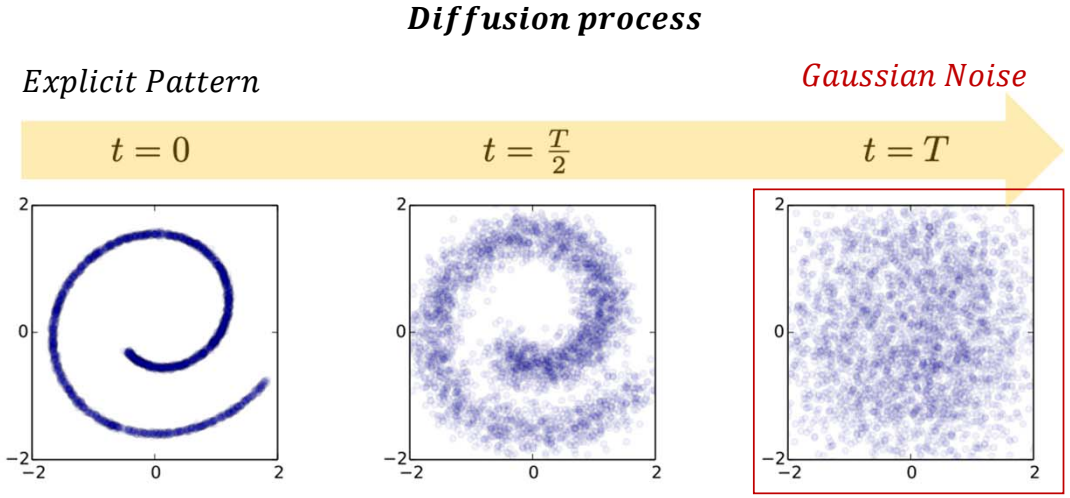
Diffusion Model Overview

From *Deep Unsupervised Learning using Nonequilibrium Thermodynamics*(2015, *ICML*)

➢ Diffusion = '확산'



$q\left(\mathbf{x}^{(0\cdots T)}\right)$



- 물리 통계 동역학("*Thermodynamics*")에서 특정한 물질(액, 기체)이 조금씩 번지며 같은 농도로 바뀌는 현상
- 물질들의 특정한 분포가 서서히 와해되는 과정
- *Deep Unsupervised Learning using Nonequilibrium Thermodynamics*(2015, *ICML*)에서 비지도학습을 위한 방법론으로 첫 활용

- 특정한 데이터의 패턴이 서서히 반복적인 과정을 거쳐 와해되는 과정("농도가 균일해지는")을 '*Diffusion process*'라 명명

Diffusion Model Overview

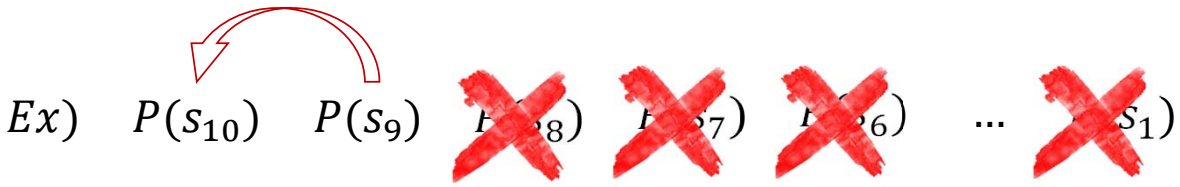
➢ Markov Chain

- **Markov 성질**을 갖는 **이산 확률과정**

✓ **Markov 성질 : "특정 상태의 확률(t+1)은 오직 현재(t)의 상태에 의존한다"**

✓ **이산 확률과정 : 이산적인 시간(0초, 1초, 2초, ..) 속에서의 확률적 현상**

$$P[s_{t+1}|s_t] = \mathrm{P}[s_{t+1}|s_1, .., s_t]$$



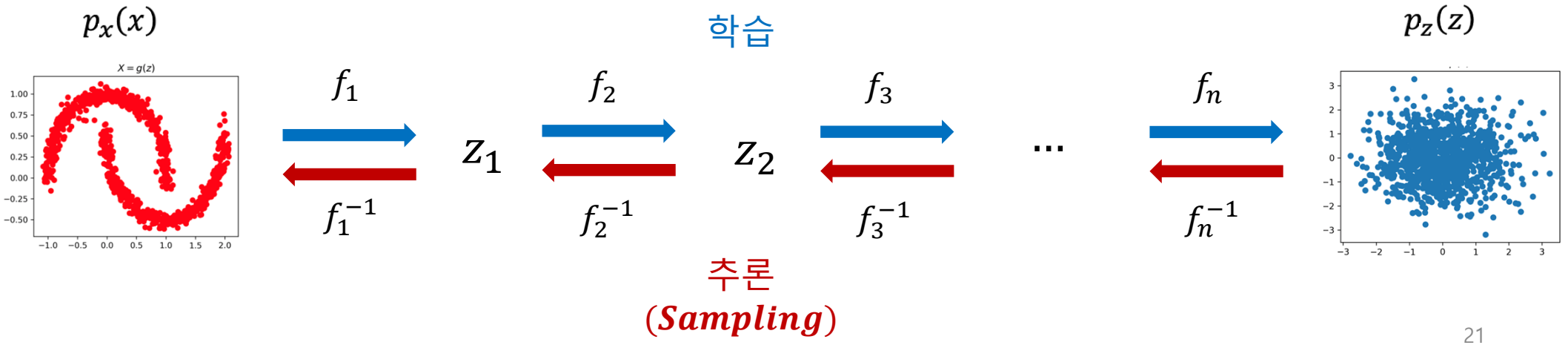
✓ **예 : "내일의 날씨는 오늘의 날씨만 보고 알 수 있다." (내일의 날씨는 오로지 오늘의 날씨 만을 조건부로 하는 확률적 과정)**

Diffusion Model Overview

➢ Normalizing Flow

- 심층 신경망 기반 확률적 생성 모형 중 하나
- 잠재 변수(z) 기반 확률적 생성모형으로서, 잠재 변수(z) 획득에 '변수 변환' 공식을 활용

✓ 변수변환 공식 $$p_x(x) = p_z(z)\left|\frac{dz}{dx}\right|$$

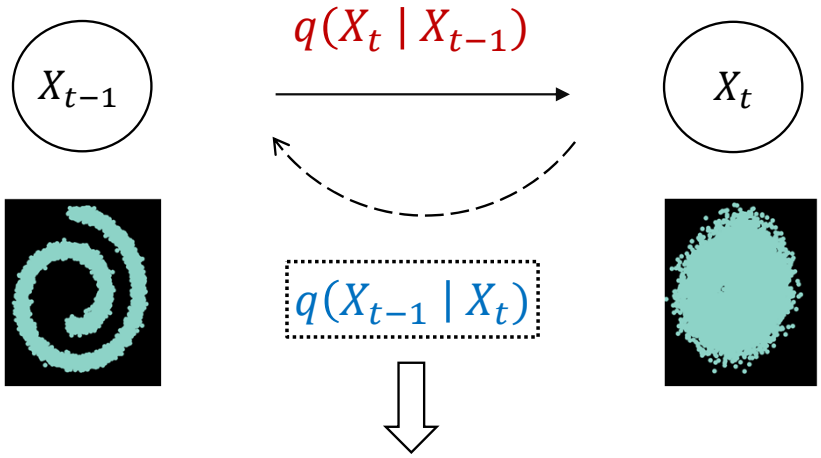


Diffusion Model Overview

➢ Diffusion Model

- **Diffusion model**은 Generative model로서 **학습된 데이터의 패턴을 생성**해내는 역할을 함
- **패턴 생성 과정을 학습하기 위해** 고의적으로 **패턴을 무너트리고(Noising),** 이를 다시 **복원하는 조건부 PDF를 학습(Denoising)**

Diffusion process *Reverse process*



$q(X_t \mid X_{t-1})$로 부터는 조건부가 바뀐 $q(X_{t-1} \mid X_t)$는 Inference과정에서 활용할 수 없음

다만, $q(X_t \mid X_{t-1})$가 gaussian이면, $q(X_{t-1} \mid X_t)$도 gaussian이라는 점은 이미 증명됨 (β_t가 매우 작을 때)

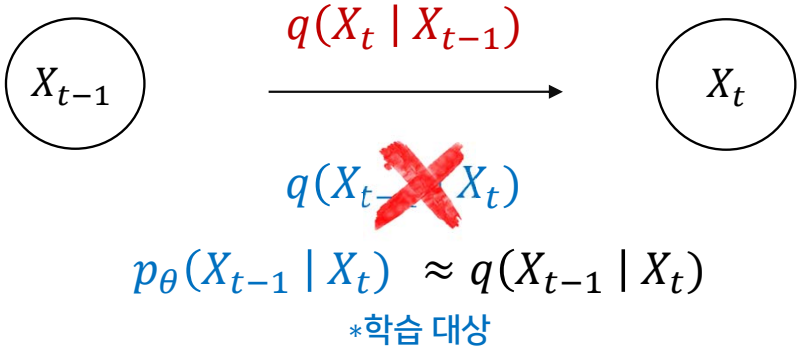
(Feller, W., 1949)

Diffusion Model Overview

➢ Diffusion Model

- **Diffusion model**은 Generative model로서 **학습된 데이터의 패턴을 생성**해내는 역할을 함
- **패턴 생성 과정을 학습하기 위해** 고의적으로 **패턴을 무너트리고(Noising),** 이를 다시 **복원하는 조건부 PDF를 학습(Denoising)**

$Diffusion\ process$ $Reverse\ process$



✓ $p_\theta(X_{t-1} \mid X_t)$ 를 상정해 $q(X_{t-1} \mid X_t)$ 를 approximation

✓ 따라서 Diffusion model은 $p_\theta(X_{t-1} \mid X_t) \approx q(X_{t-1} \mid X_t)$ 되도록 학습

Diffusion Model Overview

➢ Diffusion Model

- **Diffusion model**은 Generative model로서 **학습된 데이터의 패턴을 생성**해내는 역할을 함
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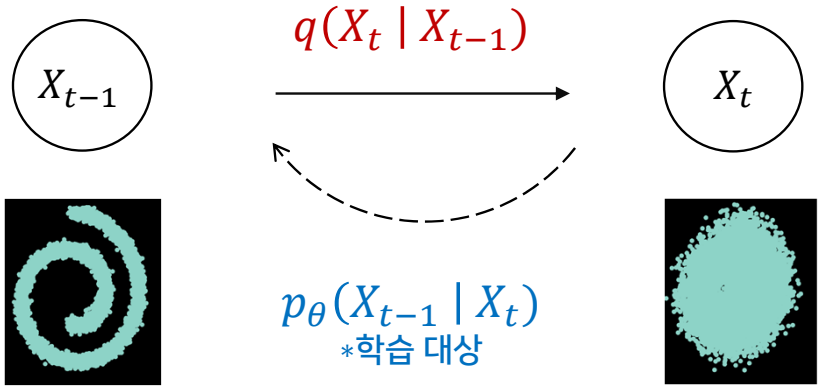


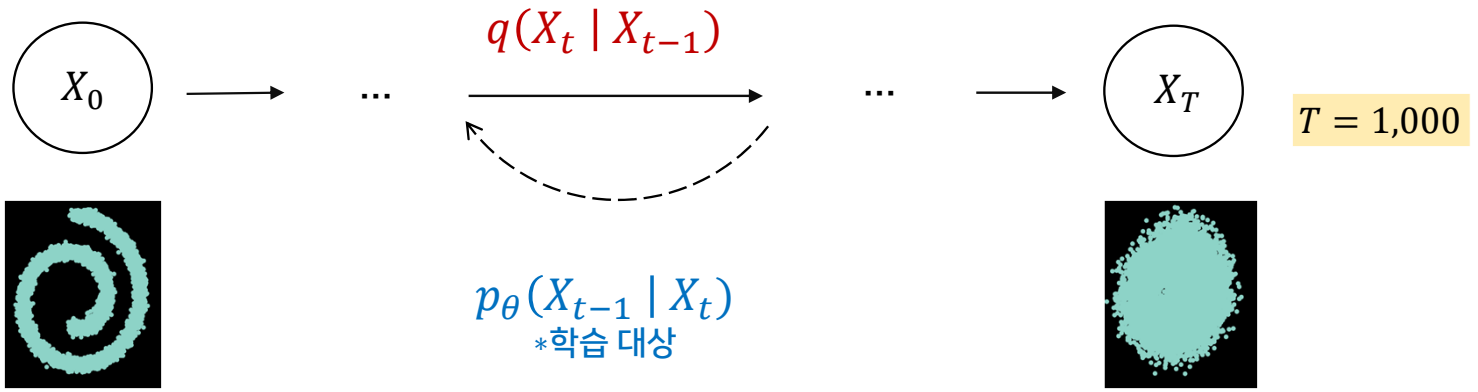
✓ 하지만 이 변화(Noising, Denoising)를 **하나의 단일 step transformation으로 학습하는 것은 매우 어려운 과제**

Diffusion Model Overview

➢ Diffusion Model

- **Diffusion model**은 Generative model로서 **학습된 데이터의 패턴을 생성**해내는 역할을 함
- **패턴 생성 과정을 학습하기 위해** 고의적으로 **패턴을 무너트리고(Noising),** 이를 다시 **복원하는 조건부 PDF를 학습(Denoising)**

$Diffusion\ process$ $Reverse\ process$



- 2개의 각 Process(Diffusion, Reverse) 내 **변화 과정**은 **Markov Chain**으로 **매우 많은 단계로 쪼개져** 구성됨
  - ✓ $p_\theta(X_t \mid X_{t-1})$ 의 학습은 결국 **"large number** of **small perturbations"**를 추정(estimate)하는 것

Denoising Diffusion Probabilistic Models (DDPM)

Diffusion Model : Diffusion Process

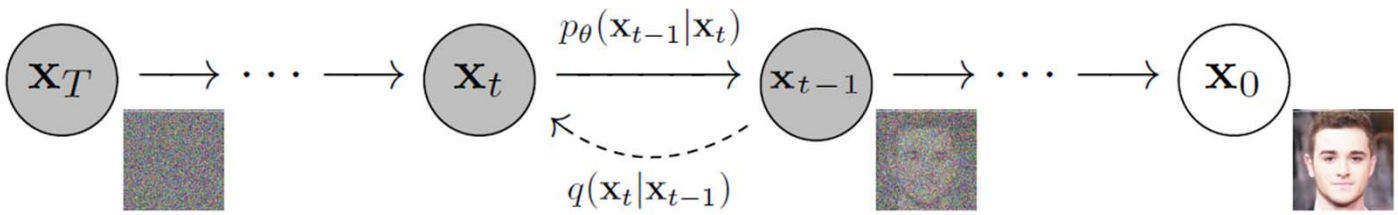


Figure 2: The directed graphical model considered in this work

Diffusion Process

- **Reverse Process**

학습

Diffusion models [53] are latent variable models of the form $p_\theta(\mathbf{x}_0) := \int p_\theta(\mathbf{x}_{0:T})\, d\mathbf{x}_{1:T}$, where $\mathbf{x}_1, \ldots, \mathbf{x}_T$ are latents of the same dimensionality as the data $\mathbf{x}_0 \sim q(\mathbf{x}_0)$. The joint distribution $p_\theta(\mathbf{x}_{0:T})$ is called the *reverse process*, and it is defined as a Markov chain with learned Gaussian transitions starting at $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$:

$$p_\theta(\mathbf{x}_{0:T}) := p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t), \qquad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) := \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \tag{1}$$

- **Forward Process**

설정

What distinguishes diffusion models from other types of latent variable models is that the approximate posterior $q(\mathbf{x}_{1:T}|\mathbf{x}_0)$, called the *forward process* or *diffusion process*, is fixed to a Markov chain that gradually adds Gaussian noise to the data according to a variance schedule $\beta_1, \ldots, \beta_T$:

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) := \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}), \qquad q(\mathbf{x}_t|\mathbf{x}_{t-1}) := \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t \mathbf{I}) \tag{2}$$

Denoising Diffusion Probabilistic Models (DDPM)

Diffusion Model : Diffusion Process

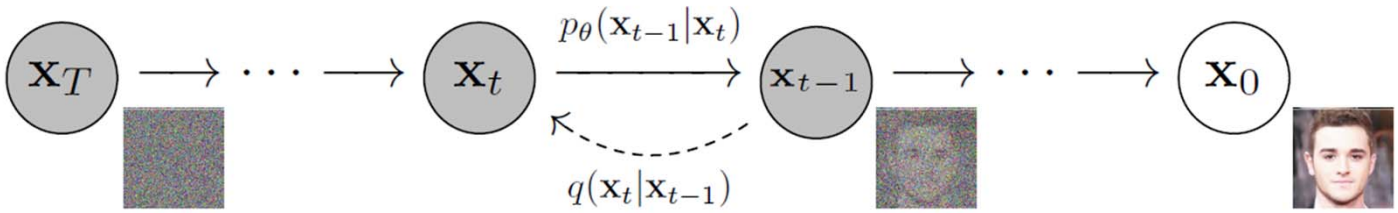


Figure 2: The directed graphical model considered in this work

Diffusion Loss

Training is performed by optimizing the usual variational bound on negative log likelihood:

$$\mathbb{E}\left[-\log p_\theta(\mathbf{x}_0)\right] \leq \mathbb{E}_q\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] = \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] =: L \quad (3)$$

The forward process variances β_t can be learned by reparameterization [33] or held constant as hyperparameters, and expressiveness of the reverse process is ensured in part by the choice of Gaussian conditionals in $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$, because both processes have the same functional form when β_t are small [53]. A notable property of the forward process is that it admits sampling $\mathbf{x}_t$ at an arbitrary timestep t in closed form: using the notation $\alpha_t := 1 - \beta_t$ and $\bar{\alpha}_t := \prod_{s=1}^{t} \alpha_s$, we have

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}) \quad (4)$$

Diffusion Model : Diffusion Process

Diffusion Loss

Efficient training is therefore possible by optimizing random terms of L with stochastic gradient descent. Further improvements come from variance reduction by rewriting L (3) as:

$$\mathbb{E}_q \Big[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0} \Big] \quad (5)$$

(See Appendix A for details. The labels on the terms are used in Section 3.) Equation (5) uses KL divergence to directly compare $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ against forward process posteriors, which are tractable when conditioned on $\mathbf{x}_0$:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}), \quad (6)$$

$$\text{where} \quad \tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t \quad \text{and} \quad \tilde{\beta}_t := \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t \quad (7)$$

Consequently, all KL divergences in Eq. (5) are comparisons between Gaussians, so they can be calculated in a Rao-Blackwellized fashion with closed form expressions instead of high variance Monte Carlo estimates.

Learning $\boldsymbol{\beta}_t$

$$\mathbb{E}_q \Big[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0} \Big]$$

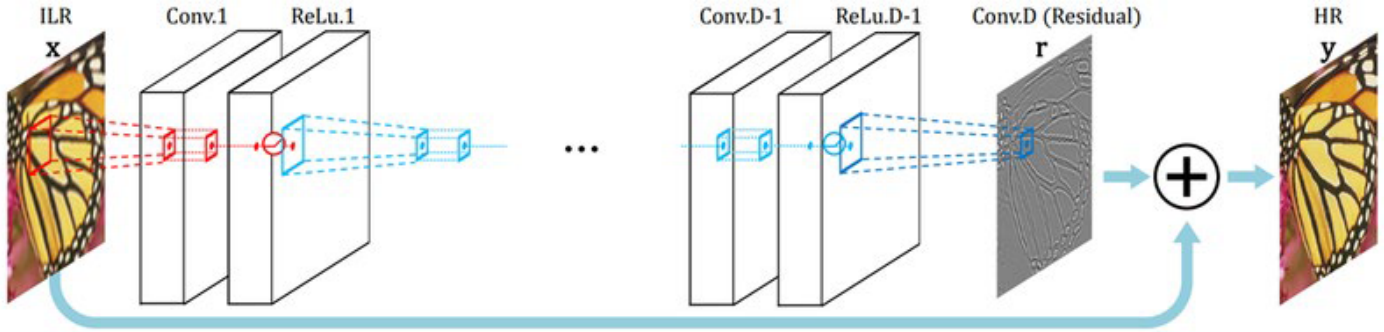
Regualization **Reconstruction**

Denoising Diffusion Probabilistic Models (DDPM)

Diffusion Model : Diffusion Process

PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc

Residual Estimation



Accurate Image Super-Resolution Using Very Deep Convolutional Networks [CVPR 2016]

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

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

예측

Residual ϵ_θ 먼저 예측

Diffusion Model : Diffusion Process

PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc

Loss Simplification

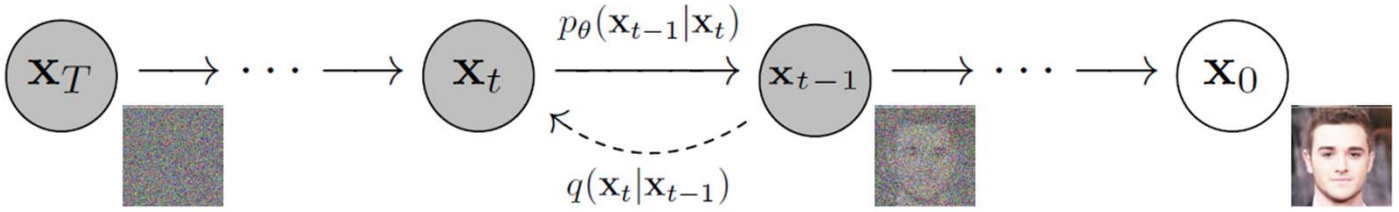
$$\mathbb{E}_q \Big[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0} \Big]$$

$$L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}} \Big[\big\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \big\|^2 \Big]$$

Loss Simplification #1 –Deleting Regularization Term

"Not to learn, just to fix β_t"

Inductive bias를 늘리는 방향



- We chose the β_t schedule from a set of constant, linear, and quadratic schedules, all constrained so that $L_T \approx 0$. We set $T = 1000$ without a sweep, and we chose a linear schedule from $\beta_1 = 10^{-4}$ to $\beta_T = 0.02$.

Diffusion Model : Diffusion Process

PR12-409, https://www.youtube.com/watch?v=1j0W_lu55nc

Loss Simplification #2 – Not to learn variance

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

$$\boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t) = \sigma_t^2 \mathbf{I}$$

$$\sigma_t^2 = \beta_t = \frac{1-\alpha_{t-1}}{1-\bar{\alpha}_t}\beta_t \quad \textbf{Or} \quad \sigma_t^2 = \beta_t$$

Loss Simplification

$$\mathbb{E}_q\left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1}\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\right]$$

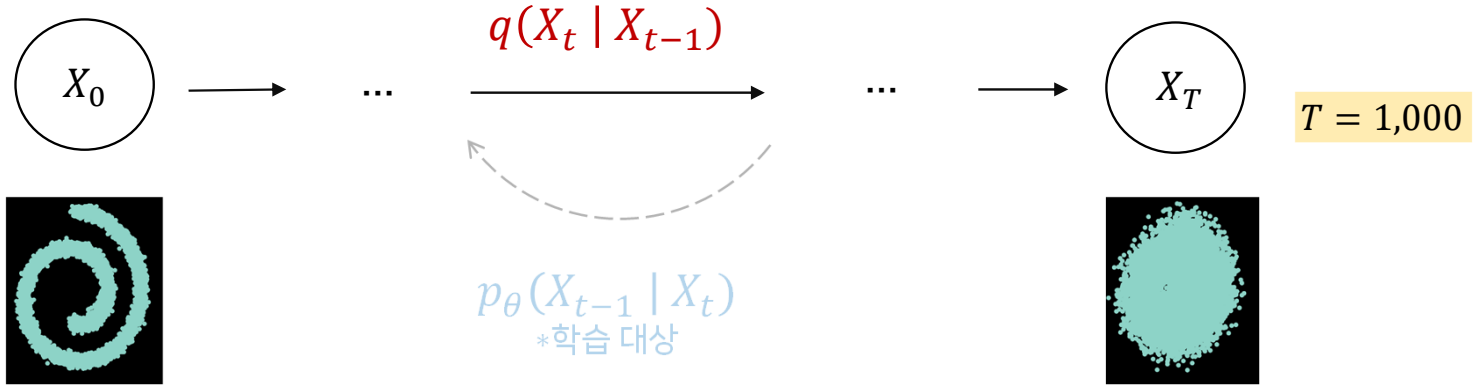
$$L_{t-1} = \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\|^2\right] + C \quad \Leftarrow \quad \boldsymbol{\mu}_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)$$

$$\mathbb{E}_{\mathbf{x}_0, \boldsymbol{\epsilon}}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2\right]$$

Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

- Diffusion process는 gaussian noise를 점진적으로 주입하는 과정
  - ✓ 조건부 Gaussian $q(X_t \mid X_{t-1})$ 의 Markov chain으로 구성됨

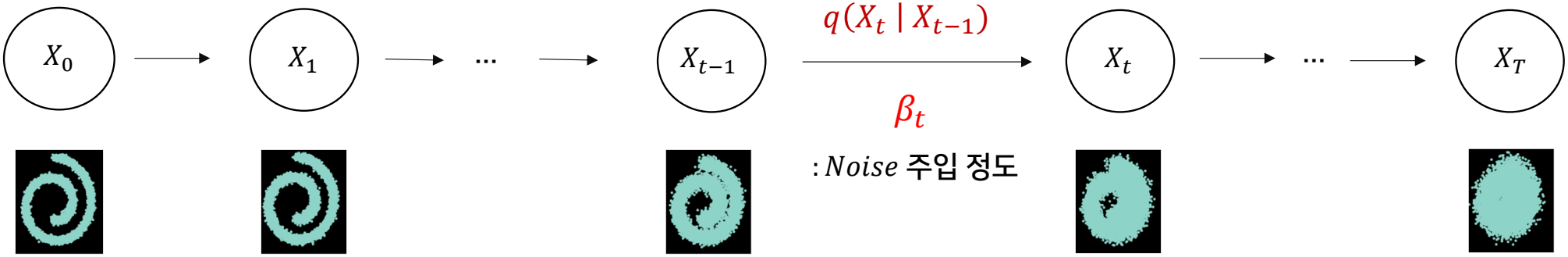


Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

- Diffusion process는 gaussian noise를 점진적으로 주입하는 과정
  - ✓ 주입되는 gaussian noise 크기는 사전적으로 정의되고, 이를 β_t로 표기

$$q(X_t \mid X_{t-1}) := N(X_t\,; \mu_{X_{t-1}}, \Sigma_{X_{t-1}}) := N\left(X_t\,; \sqrt{1-\beta_t}\,X_{t-1},\ \beta_t \cdot I\right)$$



Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

- 주입되는 gaussian noise 크기는 사전적으로 정의되고, 이를 β_t로 표기
- β_t 의 사전적 정의(scheduling)는 크게 3가지를 고려함
  - ✓ Linear schedule
  - ✓ Quad schedule
  - ✓ Sigmoid schedule

o Code Example

```
def make_beta_schedule(schedule='linear', n_timesteps=1000, start=1e-4, end=0.02):
    if schedule == 'linear':
        betas = torch.linspace(start, end, n_timesteps)
    elif schedule == "quad":
        betas = torch.linspace(start ** 0.5, end ** 0.5, n_timesteps) ** 2
    elif schedule == "sigmoid":
        betas = torch.linspace(-6, 6, n_timesteps)
        betas = torch.sigmoid(betas) * (end - start) + start
    return betas
```

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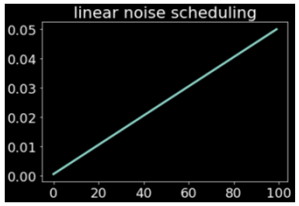
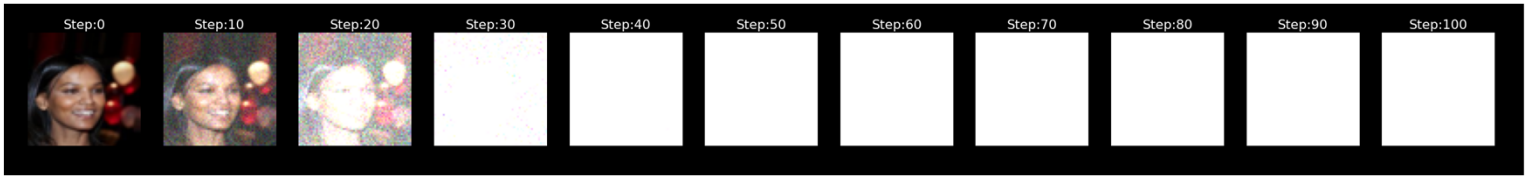
Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

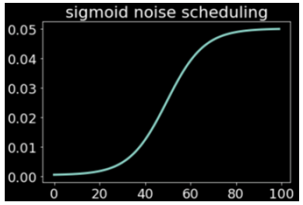
- β_t 의 사전적 정의(scheduling)는 크게 3가지를 고려함

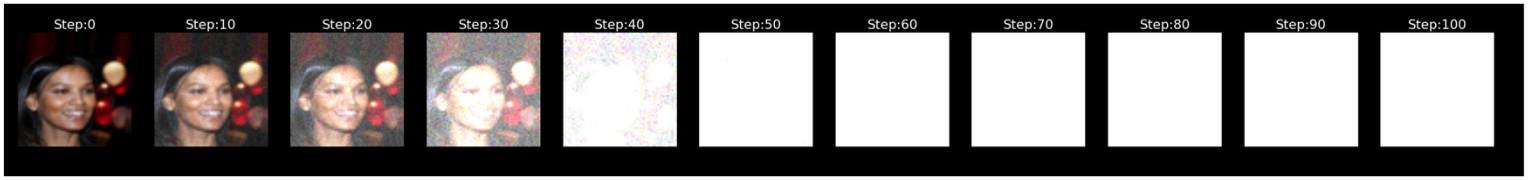
Linear scheduling



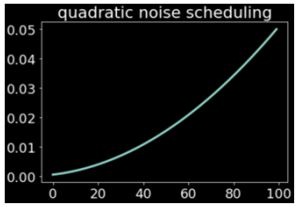


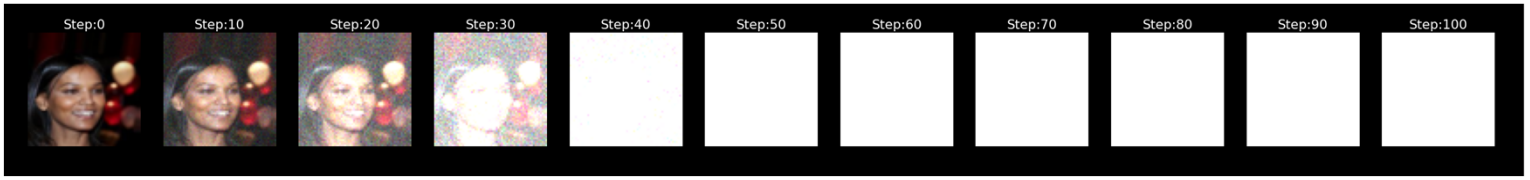
Sigmoid scheduling





Quadratic scheduling





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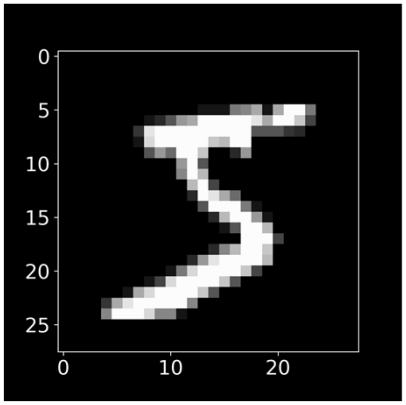
Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

- Diffusion Process GIF

Swiss-roll

MNIST



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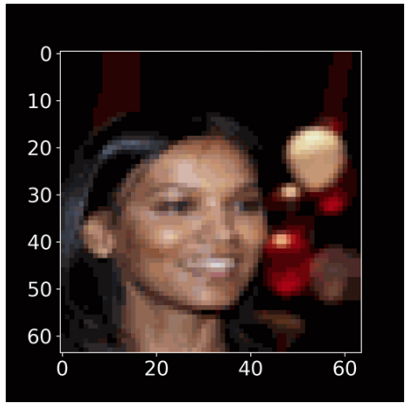


Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

- Diffusion process는 gaussian noise를 점진적으로 주입하는 과정 **(= Conditional Gaussian distribution)**

$$q(X_t \mid X_{t-1}) := N(X_t\,; \mu_{X_{t-1}}, \Sigma_{X_{t-1}}) := N\left(X_t\,; \sqrt{1-\beta_t}\,X_{t-1},\ \beta_t \cdot I\right)$$

$$= \sqrt{1-\beta_t}\,X_{t-1} + \sqrt{\beta_t}\ \epsilon_{t-1} \quad * \ \epsilon \sim N(0, I)$$ (Reparameterization trick)

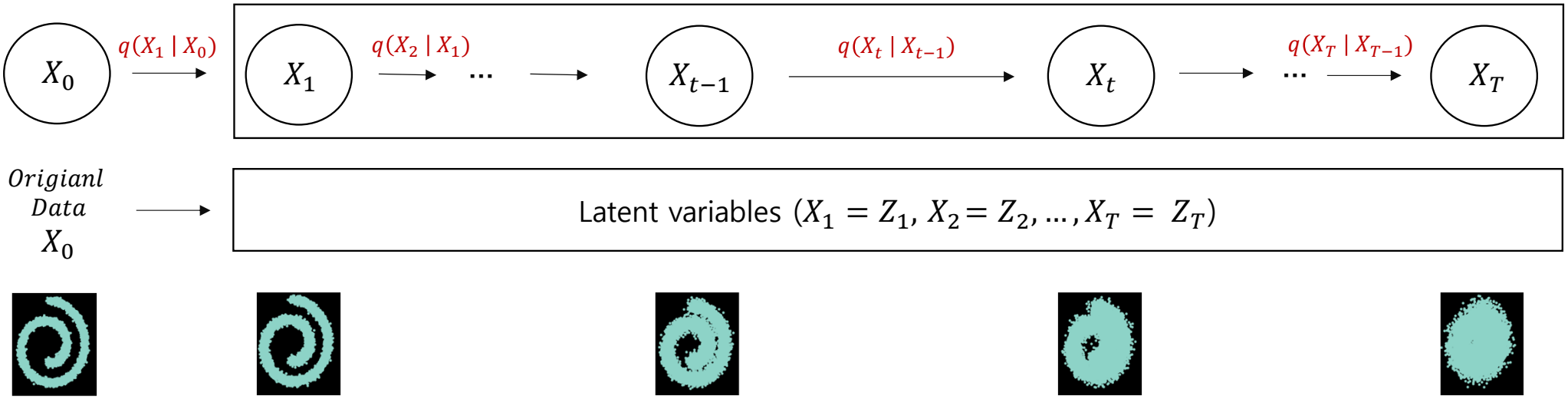
- Code Example

```
def forward_process(x_start, n_steps, noise=None):
    """
    Diffuse the data (t == 0 means diffused for 1 step)

    x_start:tensor = dataset at start step(X_0)
    n_steps:int = the number of convert iterations in diffusion process
    noise:scheduled noise set
    """
    x_sequence = [x_start] # initial 'x_seq' which is filled with origianl data at first.
    for n in range(n_steps):

        beta_t = noise[n]
        x_t_1 = x_sequence[-1]
        epsilon_t_1 = torch.rand_like(x_t_1)

        x_t = (torch.sqrt(1-beta_t) * x_t_1) + (torch.sqrt(beta_t) * epsilon_t_1)
        x_sequence.append(x_t)

    return x_seq
```

Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

- Diffusion process는 점진적으로 단계적 gaussian noise를 갖는 다수의 latent variable($X_1, X_2, \dots, X_T$)를 획득
- 다수의 latent variable($X_1, X_2, \dots, X_T$)를 상정한다는 점에서 Hierarchical VAE와 유사한 접근



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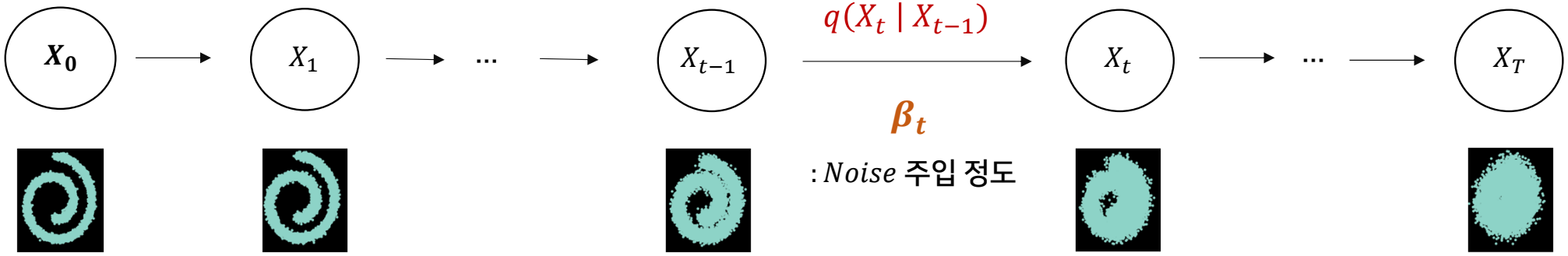
Diffusion Model : Diffusion Process

❑ Phase 1 : Diffusion Forward Process

- Diffusion process는 Contitioanl Gaussian의 joint-distribution으로서, $\boldsymbol{X_0}$**를 조건부로 latent variables(**$X_{1:T}$**)를 생성해내는 과정**

  ✓ 가장 마지막 $latent\ variable(X_T = Z_T)$로 $pure\ isotropic\ gaussain$을 획득

$$q(X_{1:T} \mid \boldsymbol{X_0}) \coloneqq \prod_{t=1}^{T} q(X_t \mid X_{t-1}), \qquad q(X_t \mid X_{t-1}) \coloneqq N(X_t\ ;\ \mu_{X_{t-1}}, \Sigma_{X_{t-1}}) \coloneqq N\left(X_t\ ; \sqrt{1-\beta_t}\, X_{t-1},\ \beta_t \cdot I\right)$$



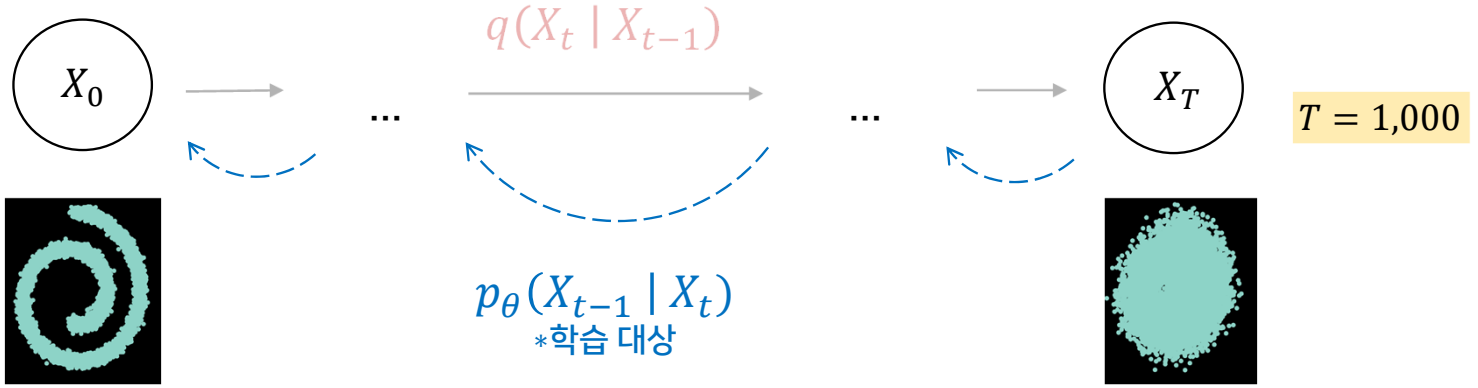
Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process

- **Diffusion model**은 Generative model로서 **학습된 데이터의 패턴을 생성**해내는 역할을 함
- **패턴 생성 과정을 학습하기 위해** 고의적으로 **패턴을 무너트리고(Noising),** 이를 다시 **복원하는 조건부 pdf를 학습함(Denoising)**

$Diffusion\ process$ $Reverse\ process$

- Reverse process는 Diffusion process의 역 과정(Denoising)을 **학습**



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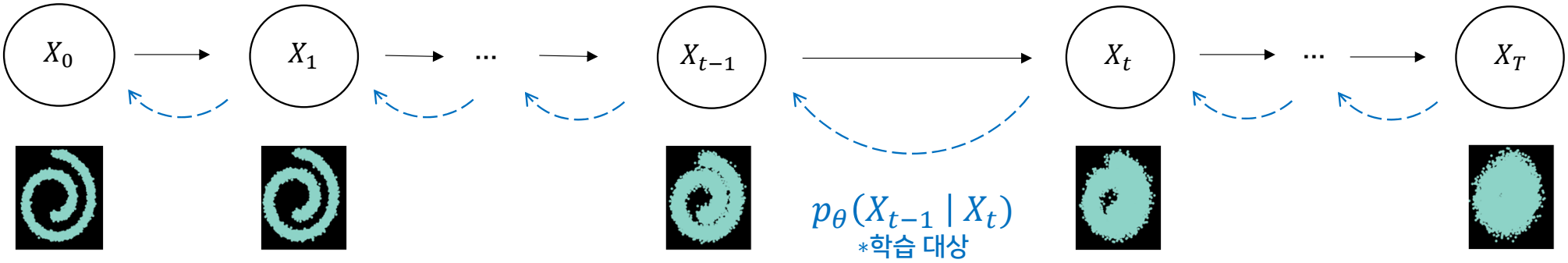
Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process

- Reverse process는 Diffusion process의 역(reverse) 과정으로, **gaussian noise를 제거**해가며 특정한 패턴을 만들어가는 과정

$$p_\theta(X_{0:T}) := p(X_T)\prod_{t=1}^{T} p_\theta(X_{t-1} \mid X_t), \qquad p_\theta(X_{t-1} \mid X_t) := N(X_{t-1}; \mu_\theta(X_t, t), \Sigma_\theta(X_t, t))$$

학습 대상
$(mean\ \&\ variance\ function)$



Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process

- Reverse process는 Diffusion process의 역(reverse) 과정으로, **gaussian noise를 제거**해가며 특정한 패턴을 만들어가는 과정

$$p_\theta(X_{0:T}) \coloneqq p(X_T) \prod_{t=1}^{T} p_\theta(X_{t-1} \mid X_t), \qquad p_\theta(X_{t-1} \mid X_t) \coloneqq N(X_{t-1}; \mu_\theta(X_t, t), \Sigma_\theta(X_t, t))$$

학습 대상
$(mean\ \&\ variance\ function)$

- Code example

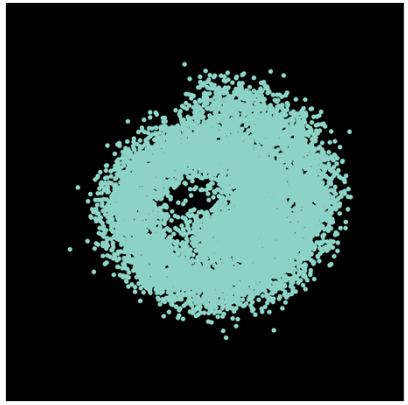
```
def p_mean_variance(model, x, t):

    # Make model prediction
    out = model(x, t.to(device))

    # Extract the mean and variance
    mean, log_var = torch.split(out, 2, dim=-1)
    var = torch.exp(log_var)
    return mean, log_var
```

Diffusion Model : Diffusion Process

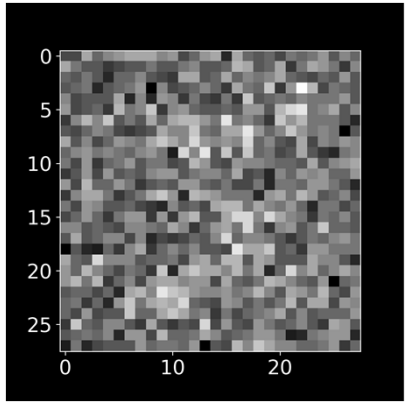
❑ Phase 2 : Diffusion Reverse Process

- Reverse process gif

Swiss-roll



MNIST



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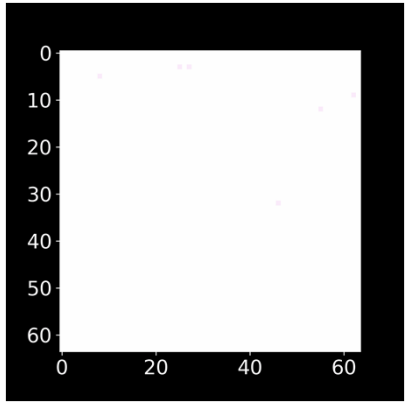


Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process Loss

$$Loss_{diffusion} := D_{KL}(q(z \mid x_0) \| P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0) \| P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

$$:= Negative\ log\ \ likelihood\ (= \mathbb{E}_{x_T \sim q(x_T \mid x_0)}[-\log p_\theta(x_0)])$$

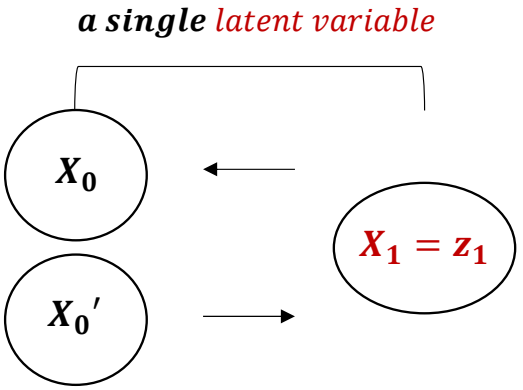
- Diffusion의 Loss는 VAE와 비교 이해 가능
- 자세한 도출 과정 참고 Blog "[논문공부] Denoising Diffusion Probabilistic Models (DDPM) 설명 (Blue collar Developer)"

Diffusion Model : Diffusion Process

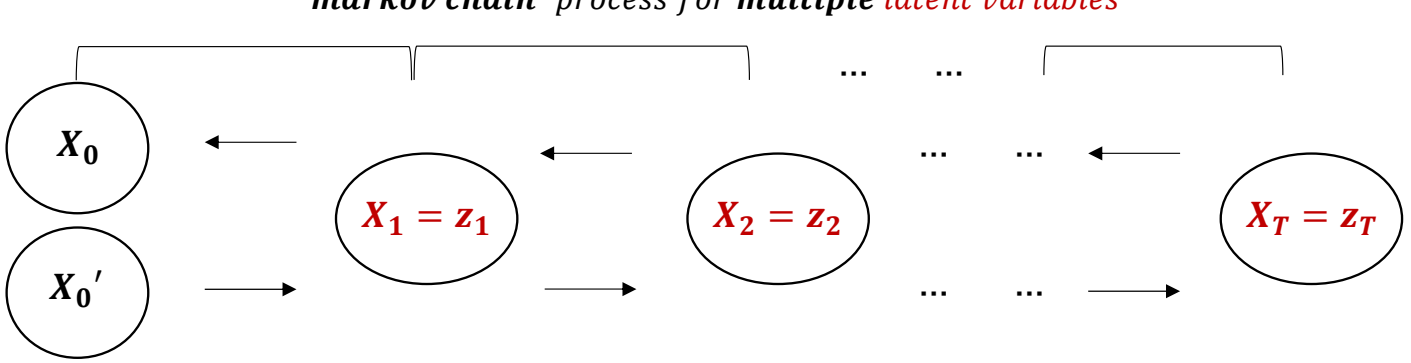
❑ Phase 2 : Diffusion Reverse Process Loss

- VAE와 Diffusion의 구조 비교

✓ VAE



✓ Diffusion

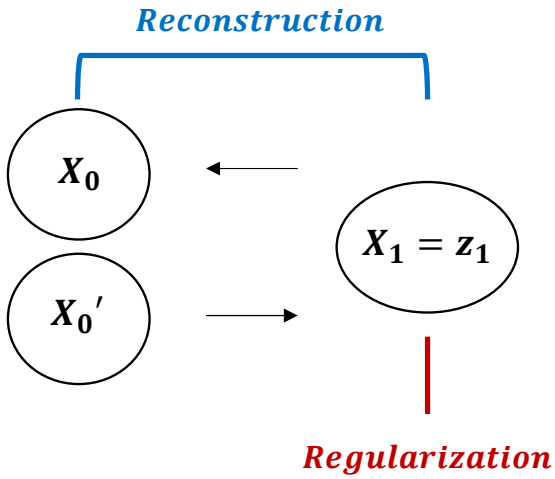


Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process Loss

- VAE와 Diffusion의 구조 비교

✓ VAE



Regularizer on Encoder *Reconstruction on Decoder*

$$Loss_{VAE} = D_{KL}(q(z \mid x) \| p_\theta(z)) - E_{z \sim q(z|x)}[\log P_\theta(x \mid z)]$$

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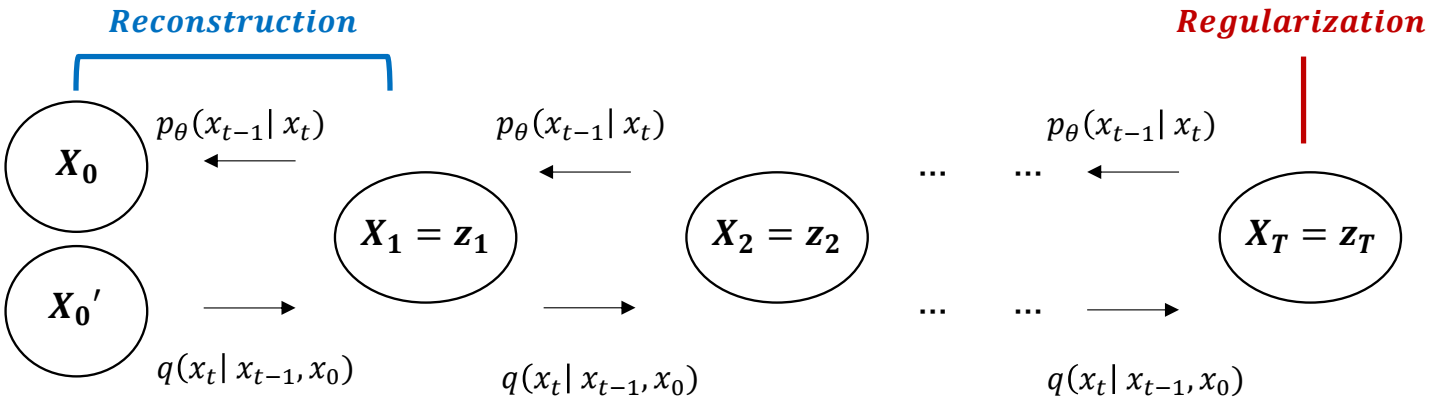
Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process Loss

- VAE와 Diffusion의 구조 비교

✓ Diffusion



$$Loss_{Diffusion} = D_{KL}(q(z \mid x_0) \| P_\theta(x_0 \mid z)) - E_{z\sim q(z|x)}[\log P_\theta(z)]$$

$$= p_\theta(x_{t-1} \mid x_t)$$

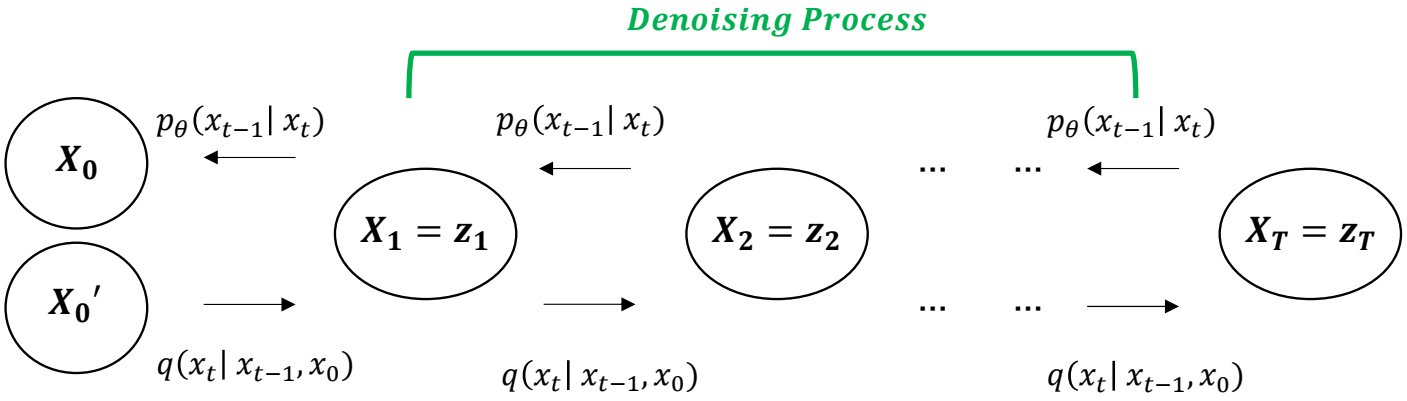
Regularization — Reconstruction

Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process Loss

- VAE와 Diffusion의 구조 비교

✓ Diffusion



$$Loss_{Diffusion} = D_{KL}(q(z \mid x_0) \| P_\theta(x_0 \mid z)) - E_{z\sim q(z|x)}[\log P_\theta(z)]$$

$$= D_{KL}(q(z \mid x_0) \| P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0) \| P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

Denoising Process

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Diffusion Model : Diffusion Process

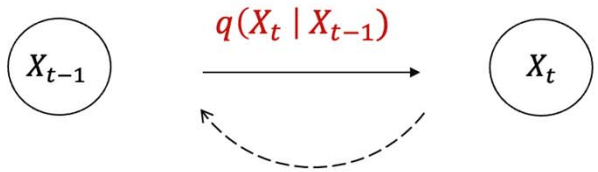
❑ Phase 2 : Diffusion Reverse Process Loss

- Diffusion model의 denoising process 학습 : $p_\theta(X_{t-1} \mid X_t) \approx q(X_{t-1} \mid X_t, X_0)$

❑ **Diffusion model**

- **Diffusion model**은 Generative model로서 **학습된 데이터의 패턴을 생성**해내는 역할을 함
- **패턴 생성 과정을 학습하기 위해** 고의적으로 **패턴을 무너트리고(Noising),** 이를 다시 **복원하는 조건부 PDF를 학습(Denoising)**

Diffusion process *Reverse process*



$q(X_{t-1} \mid X_t, X_0)$

$p_\theta(X_{t-1} \mid X_t) \approx \mathrm{q}(\mathrm{X_{t-1}} \mid \mathrm{X_t}, X_0)$

*학습 대상

✓ $p_\theta(X_{t-1} \mid X_t)$ 를 상정해 $\mathrm{q}(\mathrm{X_{t-1}} \mid \mathrm{X_t}, \mathrm{X_0})$ 를 approximation

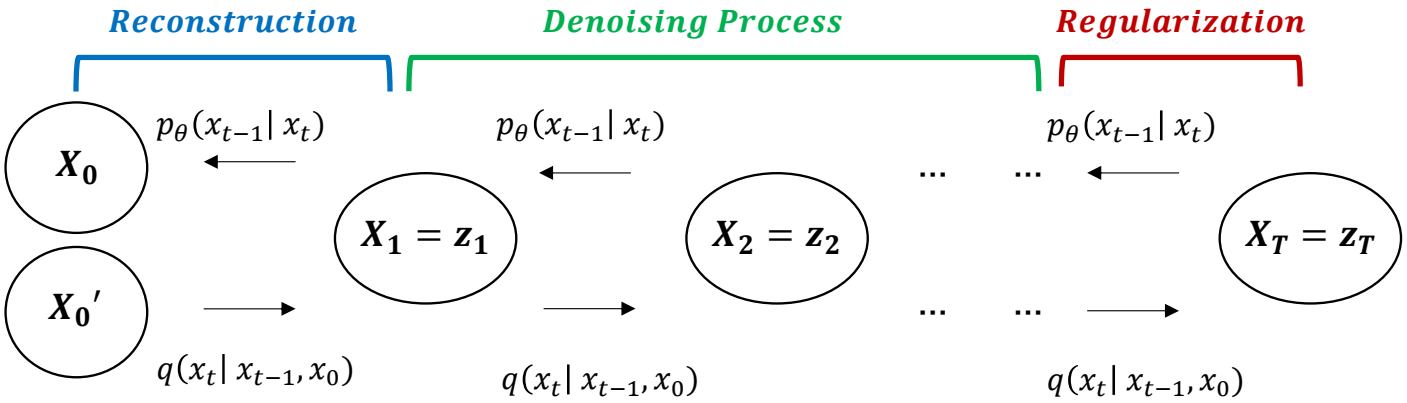
✓ 따라서 Diffusion model은 $p_\theta(X_{t-1} \mid X_t) \approx \mathrm{q}(\mathrm{X_{t-1}} \mid \mathrm{X_t}, X_0)$ 되도록 학습

Diffusion Model : Diffusion Process

❑ Phase 2 : Diffusion Reverse Process Loss

- VAE와 Diffusion의 구조 비교

✓ Diffusion



$$Loss_{Diffusion} = D_{KL}(q(z \mid x_0) \| P_\theta(x_0 \mid z)) - E_{z\sim q(z|x)}[\log P_\theta(z)]$$

$$= D_{KL}(q(z \mid x_0) \| P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0) \| P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

Regularization　　Denoising Process　　Reconstruction

Diffusion Model : Diffusion Process

- Phase 2 : Diffusion Reverse Process Loss

Regularizer on Encoder *Reconstruction on Decoder*

$$Loss_{VAE} = D_{KL}(q(z \mid x) \| p_\theta(z)) - E_{z\sim q(z|x)}[\log P_\theta(x \mid z)]$$

$$Loss_{Diffusion} = D_{KL}(q(z \mid x_0) \| P_\theta(x_0 \mid z)) - E_{z\sim q(z|x)}[\log P_\theta(z)]$$

$$= D_{KL}(q(z \mid x_0) \| P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0) \| P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

Regularization *Denoising Process* *Reconstruction*

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DDPM

- Choose the **variances β_t of the forward process** and the **model architecture** and **Gaussian distribution parameterization of the reverse process**.
- Establish **a new explicit connection between diffusion models and denoising score matching** (Section 3.2) that leads to a simplified, weighted variational bound objective for diffusion models (Section 3.4).
- Ultimately, our model design is justified by **simplicity** and **empirical** results (Section 4).

$$Loss_{Diffusion} = D_{KL}(q(z \mid x_0) \| P_\theta(x_0 \mid z)) - E_{z\sim q(z|x)}[\log P_\theta(z)]$$

$$= D_{KL}(q(z \mid x_0) \| P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0) \| P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

Regularizer on Encoder ***Denoising Process*** ***Reconstruction on Decoder***

DDPM에서는 ***Loss***가 굉장히 간단한 식으로 정의됨

$$Loss_{DDPM} = \mathbb{E}_{x_0,\epsilon}\left[\left|\epsilon - \epsilon_\theta\left(\sqrt{\tilde{\alpha}_t} + \sqrt{1-\tilde{\alpha}_t}\epsilon, t\right)\right|^2\right]$$

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DDPM

❑ Forward Process and L_T

We ignore the fact that the forward process variances β_t are learnable by reparameterization and instead fix them to constants (see Section 4 for details). Thus, in our implementation, the approximate posterior q has no learnable parameters, so L_T is a constant during training and can be ignored.

1. 학습 목적식에서 ***Regularization*** **term** 제외

✓ 굳이 학습시키지 않아도 fixed noise scheduling으로 필요한 'isotropic gaussian' 획득 가능하기 때문

$$Loss_{Diffusion} = D_{KL}(q(\cdot)\|P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0)\|P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

Regularization *Denoising Process* *Reconstruction*

Learning β_t

$$\mathbb{E}_q\left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\cdot) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\right]$$

Regualization Reconstruction

DDPM

❑ Forward Process and L_T

We ignore the fact that the forward process variances β_t are learnable by reparameterization and instead fix them to constants (see Section 4 for details). Thus, in our implementation, the approximate posterior q has no learnable parameters, so L_T is a constant during training and can be ignored.

❖ $\{\beta_1 = 10^{-4}, \dots, \beta_T = 0.02\}$ 로 Noise를 Linear하게 증가시키는 "Linear noise scheduling"을 설정할 경우

최종적인 latent variable ($Z_T = X_T$) 은 아래와 같은 분포를 갖게 됨

$$q(X_T \mid X_0) = N\left(X_T\ ;\ 0.00635 \cdot x_0, 0.99995 \cdot I\right)$$

✓ 충분한 isotropic gaussian을 확보할 수 있다고 주장함

Learning β_t

$$\mathbb{E}_q\Big[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1}\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\Big]$$

Regualization

Reconstruction

DDPM

- Reverse Process and $L_{1:T-1}$

Now we discuss our choices in $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$ for $1 < t \leq T$. First, we set $\boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t) = \sigma_t^2 \mathbf{I}$ to untrained time dependent constants. Experimentally, both $\sigma_t^2 = \beta_t$ and $\sigma_t^2 = \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$ had similar results. The first choice is optimal for $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$, and the second is optimal for $\mathbf{x}_0$ deterministically set to one point. These are the two extreme choices corresponding to upper and lower bounds on reverse process entropy for data with coordinatewise unit variance [53].

Second, to represent the mean $\boldsymbol{\mu}_\theta(\mathbf{x}_t, t)$, we propose a specific parameterization motivated by the following analysis of L_t. With $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I})$, we can write:

$$L_{t-1} = \mathbb{E}_q \left[\frac{1}{2\sigma_t^2} \|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\|^2 \right] + C \tag{8}$$

where C is a constant that does not depend on θ. So, we see that the most straightforward parameterization of $\boldsymbol{\mu}_\theta$ is a model that predicts $\tilde{\boldsymbol{\mu}}_t$, the forward process posterior mean. However, we can expand Eq. (8) further by reparameterizing Eq. (4) as $\mathbf{x}_t(\mathbf{x}_0, \boldsymbol{\epsilon}) = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$ for $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$ and applying the forward process posterior formula (7):

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

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

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

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DDPM

- Reverse Proce

$$L_{t-1} - C = \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{1}{2\sigma_t^2}\left\|\tilde{\boldsymbol{\mu}}_t\left(\mathbf{x}_t(\mathbf{x}_0,\epsilon), \frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t(\mathbf{x}_0,\epsilon) - \sqrt{1-\bar{\alpha}_t}\epsilon)\right) - \boldsymbol{\mu}_\theta(\mathbf{x}_t(\mathbf{x}_0,\epsilon), t)\right\|^2\right] \tag{9}$$

Eq (9)

$$= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{1}{2\sigma_t^2}\left\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t(\mathbf{x}_0,\epsilon) - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right) - \boldsymbol{\mu}_\theta(\mathbf{x}_t(\mathbf{x}_0,\epsilon), t)\right\|^2\right] \tag{10}$$

Equation (10) reveals that μ_θ must predict $\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right)$ given $\mathbf{x}_t$. Since $\mathbf{x}_t$ is available as input to the model, we may choose the parameterization

$$\boldsymbol{\mu}_\theta(\mathbf{x}_t, t) = \tilde{\boldsymbol{\mu}}_t\left(\mathbf{x}_t, \frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t))\right) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) \tag{11}$$

where ϵ_θ is a function approximator intended to predict ϵ from $\mathbf{x}_t$. To sample $\mathbf{x}_{t-1} \sim p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is to compute $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$, where $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$. The complete sampling procedure, Algorithm 2, resembles Langevin dynamics with $\boldsymbol{\epsilon}_\theta$ as a learned gradient of the data density. Furthermore, with the parameterization (11), Eq. (10) simplifies to:

$$\mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2\right] \tag{12}$$

which resembles denoising score matching over multiple noise scales indexed by t [55]. As Eq. (12) is equal to (one term of) the variational bound for the Langevin-like reverse process (11), we see that optimizing an objective resembling denoising score matching is equivalent to using variational inference to fit the finite-time marginal of a sampling chain resembling Langevin dynamics.

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DDPM

- Reverse Process and $L_{1:T-1}$

To summarize, we can train the reverse process mean function approximator μ_θ to predict $\tilde{\mu}_t$, or by modifying its parameterization, we can train it to predict ϵ. (There is also the possibility of predicting $\mathbf{x}_0$, but we found this to lead to worse sample quality early in our experiments.) We have shown that the ϵ-prediction parameterization both resembles Langevin dynamics and simplifies the diffusion model's variational bound to an objective that resembles denoising score matching. Nonetheless, it is just another parameterization of $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$, so we verify its effectiveness in Section 4 in an ablation where we compare predicting $\boldsymbol{\epsilon}$ against predicting $\tilde{\boldsymbol{\mu}}_t$.

Algorithm 1 Training

1: **repeat**
2: $\quad \mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $\quad t \sim \text{Uniform}(\{1, \dots, T\})$
4: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: $\quad$ Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
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: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

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DDPM

- Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

$$Loss_{Diffusion} = D_{KL}(q(\cdot)\|P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0)\|P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

Regularization

Denoising Process

$$\mathbb{E}_q\left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\right]$$

Regualization

Reconstruction

DDPM

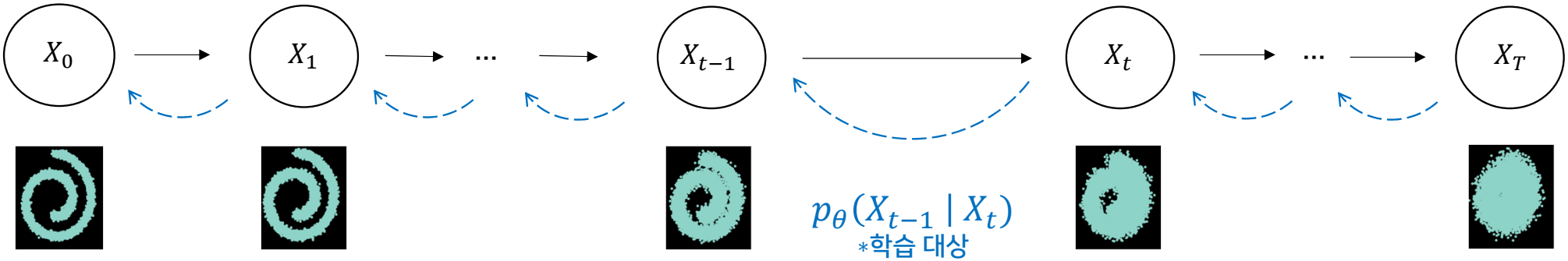
❑ Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

- Reverse process는 Diffusion process의 역(reverse) 과정으로, **gaussian noise를 제거(Denoising)**해가며 특정한 패턴을 만들어가는 과정

$$p_\theta(X_{0:T}) := p(X_T)\prod_{t=1}^{T} p_\theta(X_{t-1} \mid X_t), \qquad p_\theta(X_{t-1} \mid X_t) := N(X_{t-1}; \mu_\theta(X_t, t), \Sigma_\theta(X_t, t))$$

학습 대상
$(mean\ \&\ variance\ function)$



DDPM

❑ Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

1) $\Sigma_\theta(X_t, t)$ 의 상수화 :

✓ 학습 대상$(mean\ \&\ variance\ function)$

(1) $\mu_\theta(X_t, t) \rightarrow \mu_\theta(X_t, t)$

(2) $\Sigma_\theta(X_t, t) \rightarrow Constant\ (time\ dependent) = \sigma_t^2 \cdot I = \tilde{\beta}_t \cdot I = t$시점까지의 누적된 $noise$

- $\sigma_t^2 = \tilde{\beta}_t = \frac{1-\overline{\alpha_{t-1}}}{1-\overline{\alpha_t}}\beta_t \qquad (\overline{\alpha_t} := \prod_{s=1}^{t} \alpha_s,\ \alpha_t = 1-\beta_t)$

DDPM

❑ Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

1) $\Sigma_\theta(X_t, t)$ 의 상수화 :

- DDPM 이전

$$p_\theta(X_{0:T}) := p(X_T)\prod_{t=1}^{T} p_\theta(X_{t-1} \mid X_t), \qquad p_\theta(X_{t-1} \mid X_t) := N(X_{t-1}; \underline{\mu_\theta(X_t, t)}, \underline{\Sigma_\theta(X_t, t)})$$

학습 대상
$(mean\ \&\ variance\ function)$

- DDPM 이후

$$p_\theta(X_{0:T}) := p(X_T)\prod_{t=1}^{T} p_\theta(X_{t-1} \mid X_t), \qquad p_\theta(X_{t-1} \mid X_t) := N(X_{t-1}; \underline{\mu_\theta(X_t, t)}, \ \sigma_t^2 \cdot I)$$

학습 대상
$(mean\ function)$

DDPM

- Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

2) $\mu_\theta(x_t, t)$ 을 새롭게 정의 : Denoising matching

$$\sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0) \| P_\theta(x_{t-1} \mid x_t))$$

$$q(x_{t-1} \mid x_t, x_0) = N(x_{t-1}\,;\, \tilde{\mu}_t(x_t, x_0), \tilde{\beta}_t \cdot I)$$

$$p_\theta(x_{t-1} \mid x_t) = N(x_{t-1}\,;\, \mu_\theta(x_t, t),\ \tilde{\beta}_t \cdot I)$$

$$\mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\left\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\right\|^2\right]$$

Denoising Process

DDPM

- Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

2) $\mu_\theta(x_t, t)$ 을 새롭게 정의 : *Denoising matching*

$$\mathbf{x}_t(\mathbf{x}_0, \boldsymbol{\epsilon}) = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon} \text{ for } \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \qquad (\ \overline{\alpha_t} \coloneqq \prod_{s=1}^{t} \alpha_s\ ,\ \alpha_t = 1-\beta_t\ )$$

$\because\ q(x_t \mid x_{t-1}) := N\left(x_{t-1}; \sqrt{1-\beta_t}\, x_{t-1},\ \beta_t \cdot I\right), \qquad x_t = \sqrt{1-\beta_t}\, x_{t-1} + \sqrt{\beta_t}\ \epsilon_{t-1} \qquad * \ \epsilon \sim N(0, I)$

위에서 정의한 x_t를 아래의 식 (1)에 대입하면, 식 (2)와 같이 정리된다.

(1) $$\mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\left\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\right\|^2\right]$$

(2) $$\mathbb{E}_{\mathbf{x}_0, \boldsymbol{\epsilon}}\left[\frac{1}{2\sigma_t^2}\left\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t(\mathbf{x}_0, \boldsymbol{\epsilon}) - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right) - \boldsymbol{\mu}_\theta(\mathbf{x}_t(\mathbf{x}_0, \boldsymbol{\epsilon}), t)\right\|^2\right]$$

DDPM

- Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

2) $\mu_\theta(x_t, t)$ 을 새롭게 정의 : *Denoising matching*

(2) $$\mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{1}{2\sigma_t^2}\left\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon})-\frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right)-\boldsymbol{\mu}_\theta(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon}),t)\right\|^2\right]$$

식 (2)에 따르면, 학습할 **mean function $\boldsymbol{\mu_\theta(x_t, t)}$** 는 주어진 t 시점에 $\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{X}_t-\frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right)$ 를 예측해내야 한다.

x_t $(input)$와 t는 주어지므로, **$\boldsymbol{\mu_\theta(x_t, t)}$ 에게 남은 예측 대상은 t시점의 noise(ϵ) 뿐이다.**

따라서 아래 식 (3)과 같이 학습 모델 $\mu_\theta(x_t, t)$ 을 새롭게 정의한다.

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

DDPM

- Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

2) $\mu_\theta(x_t, t)$ 을 새롭게 정의 : *Denoising matching*

$$(2) \quad \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{1}{2\sigma_t^2}\left\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon})-\frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right)-\boldsymbol{\mu}_\theta(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon}),t)\right\|^2\right]$$

$$(3) \quad \boldsymbol{\mu}_\theta(\mathbf{x}_t,t)=\tilde{\boldsymbol{\mu}}_t\left(\mathbf{x}_t,\frac{1}{\sqrt{\bar{\alpha}_t}}\left(\mathbf{x}_t-\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t)\right)\right)=\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t-\frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,t)\right)$$

식 (2)와 식 (3)을 조합하면 아래 식 (4)와 같은 새로운 목적식이 정의된다.

$$(4) \quad \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon}-\boldsymbol{\epsilon}_\theta\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon},t\right)\right\|^2\right]$$

DDPM

- Reverse Process and $L_{1:T-1}$

2. ***Denoising Process*** 의 목적식 재구성

2) $\mu_\theta(x_t, t)$ 을 새롭게 정의 : *Denoising matching*

$$(4) \quad \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon}-\boldsymbol{\epsilon}_\theta\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon},t\right)\right\|^2\right]$$

결국 DDPM model(ϵ_θ)이 학습해야 하는 것은 주어진 t 시점의 gaussian noise(ϵ) 가 된다.

이처럼 각 시점의 다양한 scale의 gaussian noise를 예측해, denoising에 활용하고자 하는 것이 DDPM의 지향점이다.

최종적으로는 계수 term을 제외한 아래 식 (5)의 Loss를 사용

$$(5) \quad L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\left\|\boldsymbol{\epsilon}-\boldsymbol{\epsilon}_\theta\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon},t\right)\right\|^2\right]$$

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DDPM

❑ DDPM Loss

$$Loss_{Diffusion} = D_{KL}(q(z \mid x_0) \| P_\theta(x_0 \mid z)) - E_{z\sim q(z|x)}[\log P_\theta(z)]$$

$$= D_{KL}(q(z \mid x_0) \| P_\theta(z)) + \sum_{t=2} D_{kL}(q(x_{t-1} \mid x_t, x_0) \| P_\theta(x_{t-1} \mid x_t)) - E_q[\log P_\theta(x_0 \mid x_1)]$$

Regularizer on Encoder ***Denoising Process*** ***Reconstruction on Decoder***

DDPM에서는 ***Loss***가 굉장히 간단한 식으로 정의됨

(5) $$Loss_{DDPM} = \mathbb{E}_{x_0,\epsilon}\left[\left|\epsilon - \epsilon_\theta\left(\sqrt{\tilde{\alpha}_t} + \sqrt{1-\tilde{\alpha}_t}\epsilon, t\right)\right|^2\right]$$

Experimental Results

❑ Sample quality

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 Σ)	7.67 ± 0.13	13.51	≤ 3.70 (3.69)
Ours (L_{simple})	9.46 ± 0.11	**3.17**	≤ 3.75 (3.72)

- DDPM의 FID score는 3.17로서 Unconditional 생성모형 중 가장 높은 sample quality를 보임
- 계수 Term을 제외한 경우($Ours : L_{simple}$)는 제외하지 않은 경우 (Ours : L)에 비해 NLL이 높지만, Sample quality(FID score)는 월등히 높음을 확인할 수 있음

Experimental Results

❑ Sample quality

Table 2: Unconditional CIFAR10 reverse process parameterization and training objective ablation. Blank entries were unstable to train and generated poor samples with out-of-range scores.

	Objective	IS	FID
	$\tilde{\mu}$ prediction (baseline)		
(1)	L, learned diagonal Σ	7.28 ± 0.10	23.69
	L, fixed isotropic Σ	8.06 ± 0.09	13.22
(2)	$\|\tilde{\mu} - \tilde{\mu}_\theta\|^2$	–	–
	ϵ prediction (ours)		
(3)	L, learned diagonal Σ	–	–
	L, fixed isotropic Σ	7.67 ± 0.13	13.51
(4)	$\|\tilde{\epsilon} - \epsilon_\theta\|^2$ (L_{simple})	$\mathbf{9.46 \pm 0.11}$	**3.17**

(1) $$\mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\left\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\right\|^2\right]$$

(2) $$\mathbb{E}_q\left[\left\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\right\|^2\right]$$

(3) $$\mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\epsilon - \epsilon_\theta\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t\right)\right\|^2\right]$$

(4) $$\mathbb{E}_{t,\mathbf{x}_0,\epsilon}\left[\left\|\epsilon - \epsilon_\theta\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t\right)\right\|^2\right]$$

매우 불안정한 학습 및 성능이 매우 악화된 경우, "–" 로 표기

- $\tilde{\mu}$ 예측 목적식의 경우, Fixed variance를 사용했을 때, 성능이 향상됨. 다만, 목적식의 간단화(simplification)에서는 성능이 매우 악화됨
- ϵ 예측 목적식의 경우, Fixed variance를 사용할 경우 & 목적식의 간단화를 적용할 경우 성능이 크게 향상됨

Experimental Results

❑ Sample quality

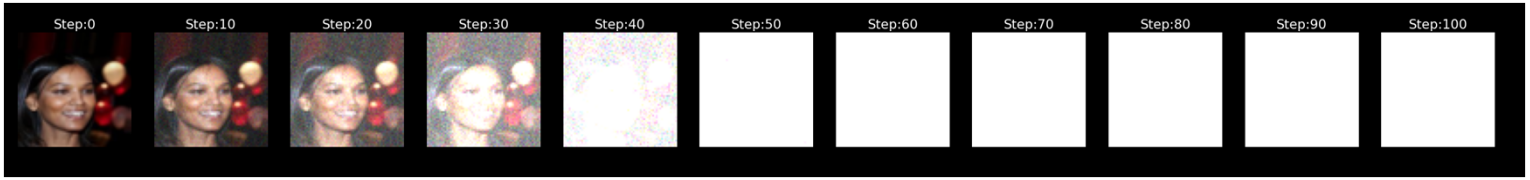
	ϵ prediction (ours)		
(3)	L, learned diagonal Σ	–	–
(3)	L, fixed isotropic Σ	7.67±0.13	13.51
(4)	$\|\tilde{\epsilon} - \epsilon_\theta\|^2$ (L_{simple})	**9.46±0.11**	**3.17**

Coefficient term

(3) $$\mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\epsilon-\epsilon_\theta\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\epsilon,t\right)\right\|^2\right]$$

(4) $$\mathbb{E}_{t,\mathbf{x}_0,\epsilon}\left[\left\|\epsilon-\epsilon_\theta\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\epsilon,t\right)\right\|^2\right]$$

Small "t" ***Large "t"***



- 목적식 (3) : *Coefficient term* 은 t가 증가할 수록 그 값이 작아지는 경향을 갖게 됨
  - 따라서 ***Coefficient term*** **이 존재할 경우, large t 시점(더 noisy)의 Loss가 상대적으로 down-weight 되는 효과가 발생**
- **목적식 (4) : *Coefficient term* 을 제거함으로써, large t 시점(더 noisy)의 Loss 비중을 더 높일 수 있음**
  - 이를 통해 **모델이 noise가 심한 이미지(large t 시점의 상태)의 denoising에 집중하도록 유도**

Experimental Results

- Progressive generation

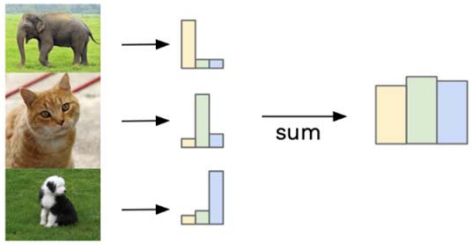
Appendix

IS socre

From blog post from 'A simple explanation of the Inception Score(David Mack)"

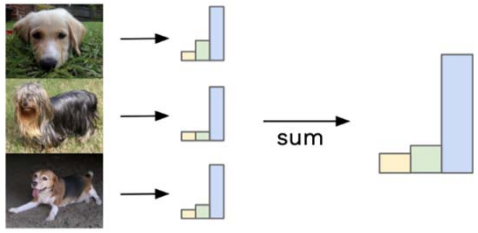
❑ Inception Score : the higher, the better

- *Improved Techniques for Training GANs(Tim Salimans, 2016)*에서 제안된 generated image sample quality 평가 지표
- Inception image classifier를 활용해 'inception'이라는 명칭을 사용함
- 2가지 특성을 통해 생성된 이미지의 품질을 평가. 아래 2가지를 만족할 수록 높은 score 획득
  - ✓ Image quality : 생성된 이미지가 명확히 object를 표현하고 있는 지(realistic?)



생성된 image들이 명확한 object를 갖는 다면,
각각의 likelihood 분포의 summation은 균일한 분포를 가질 것

  - ✓ Image diversity : 다양한 object가 생성되는 지('dog' class : {Bulldog, Poodle, ...})



생성된 image들이 다양한 object를 가질 수 있다면,
각각의 likelihood 분포의 summation은 균일하지 않은 분포를 가질 것

둘 간의 KL divergence로 Inception Score 산출

Appendix

From blog post from 'Wandb.ai"

FID score

❑ FID(Frechet Inception Distance) score : the lower, the better

- Pre-trained Image classification model을 활용해 추출한 feature representation 간의 거리(distance)를 score로 활용
  - 거리(distance)는 Frechet distance로 측정
    - Frechet distance는 곡선을 이루는 points의 위치와 순서를 고려해 두 곡선 간 유사도를 측정하는 지표

      예를 들어, 일변량 정규분포 간 Frechet distance는 아래와 같이 측정됨

$$\mathrm{d}(\mathrm{X},\mathrm{Y}) = (\mu_{\mathrm{X}} - \mu_{\mathrm{Y}})^2 + (\sigma_{\mathrm{X}} - \sigma_{\mathrm{Y}})^2$$

- Feature 정보는 후반부 layer에서 추출한 high level representation을 활용
- FID score의 계산은 아래와 같은 순서로 진행

1. $Pretrained\ image\ classification\ model\ define(ex:\ inception\ model)$
2. $Compute\ embedding(feature\ representation)$

   $2-1)\ Embedding\ of\ real\ image$

   $2-2)\ Embedding\ of\ generated\ image$
3. $Calculate\ "Frechet\ distance"\ between\ 2-1)\ and\ 2-2)$