More Generative Models

Jan 2nd, 2023

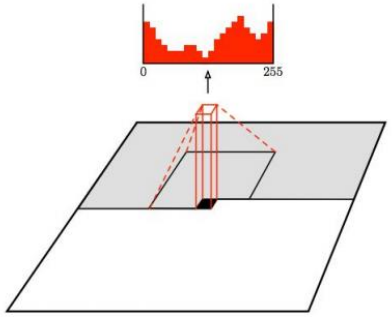
Tali Dekel

Learn the probability distribution of natural images

Generative Models Taxonomy

Explicitly density estimation

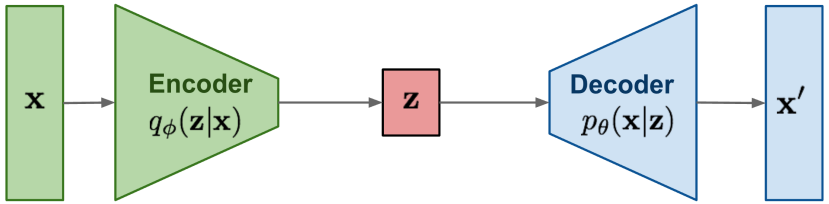
Autoregressive image generation



PixelRNN / PixelCNN

Directly maximize the log likelihood of the training data

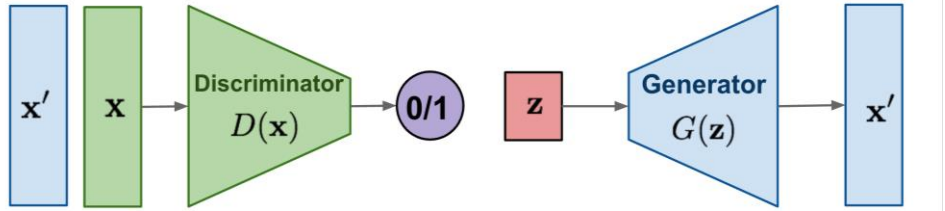
Variational Autoencoders (VAEs)



Maximize the variational lower bound of the data likelihood

Implicit density estimation

Generative Adversarial Networks (GANs)



Does not model the density function, only care about sampling

Learn the probability distribution of natural images

Generative Models Taxonomy

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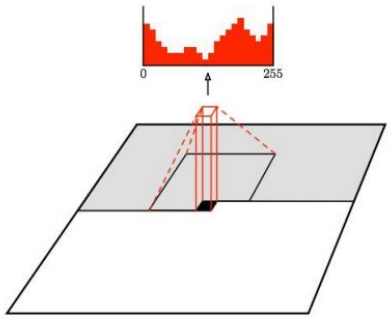
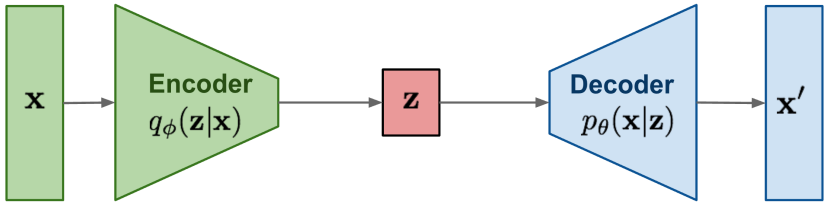


PixelRNN / PixelCNN

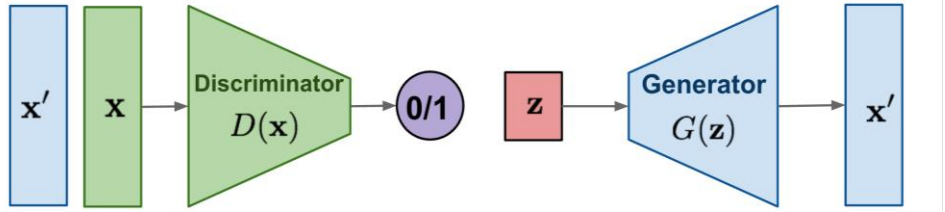
Variational Autoencoders (VAEs)



Vector Quantize - Variational Autoencoders (VQ-VAEs)

Implicit density estimation

Generative Adversarial Networks (GANs)

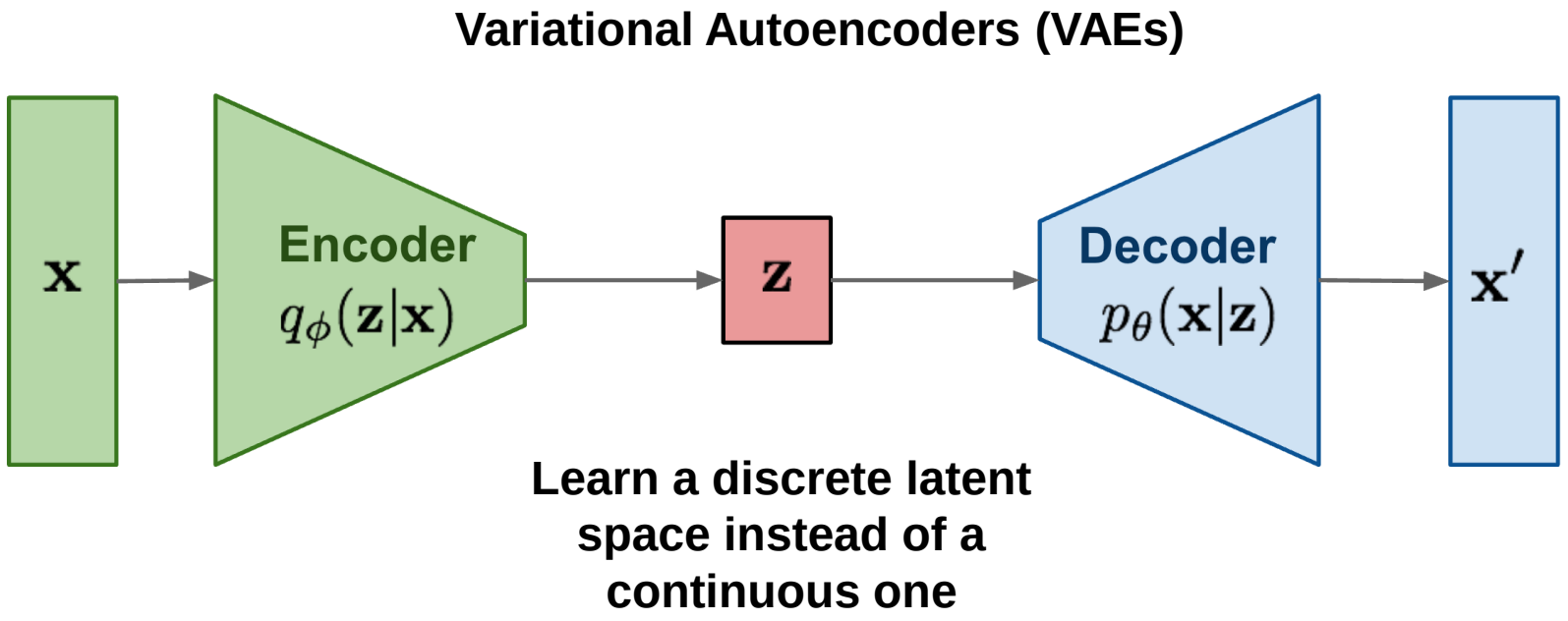


Does not model the density function, only care about sampling

Diffusion Models

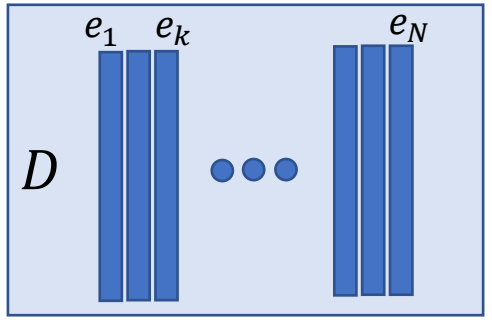
Vector Quantize - GAN (VQ-GAN)

Vector Quantize VAE (VQ-VAE)



- Discrete objects
- Discrete attributes, e.g., colors, shape, size etc’
- Algorithms and architectures that operate on discrete data

Vector Quantize VAE (VQ-VAE)



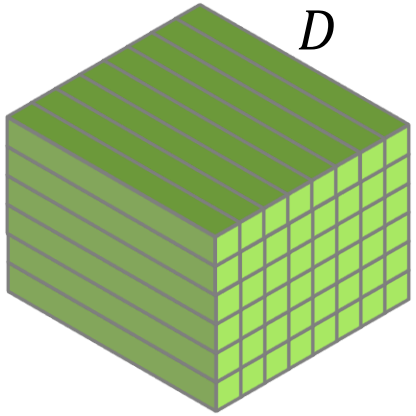
$e_k \in R^D$
$k \in (1, \ldots, N)$

Codebook (N latent codes)

x

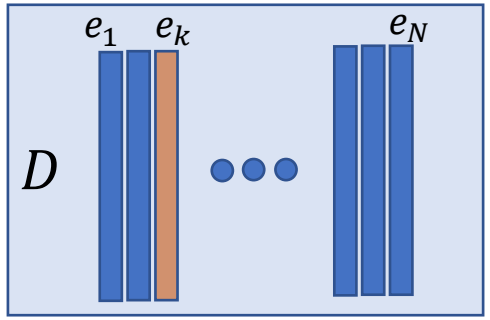
Encoder (CNN)

$z_e(x)$

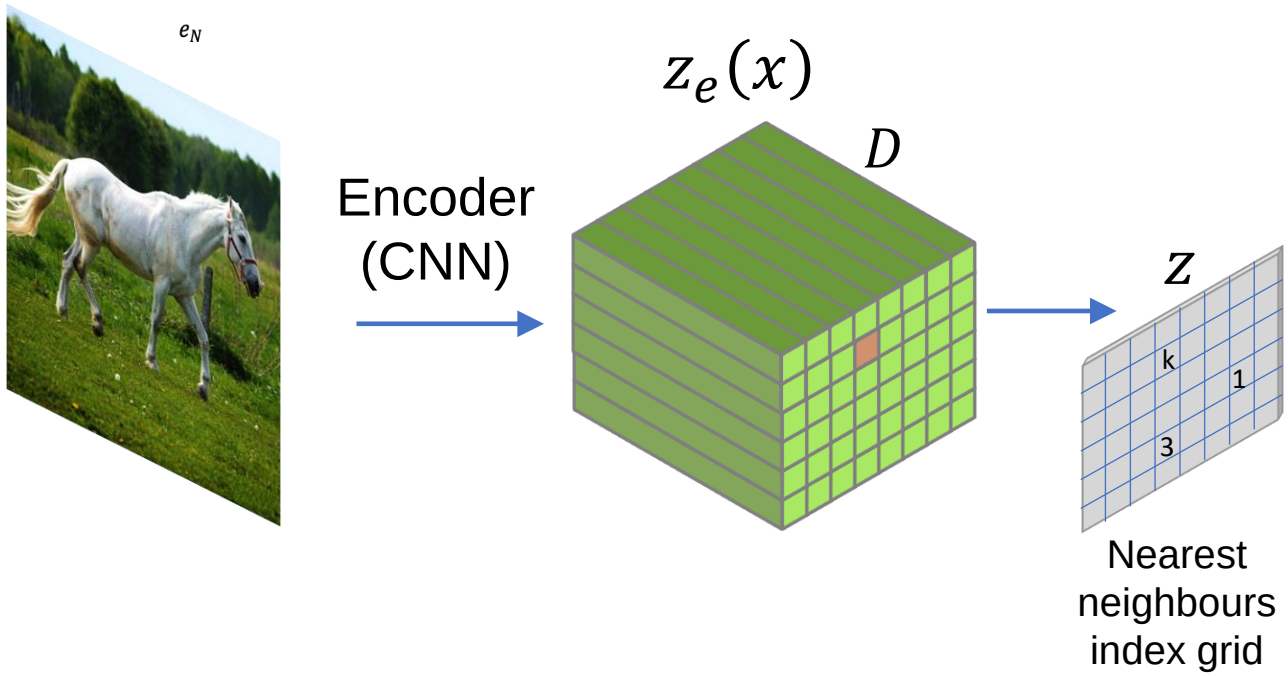


den Oord et. al, “Neural Discrete Representation Learning”,

Vector Quantize VAE (VQ-VAE)



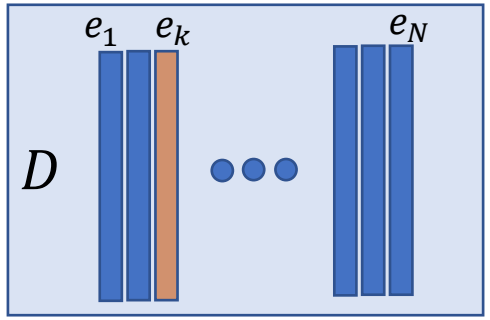
Codebook (N latent codes)



Nearest neighbours index grid

den Oord et. al, “Neural Discrete Representation Learning”, Neurips’17

Vector Quantize VAE (VQ-VAE)



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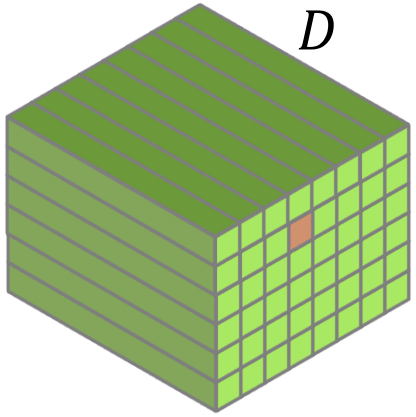
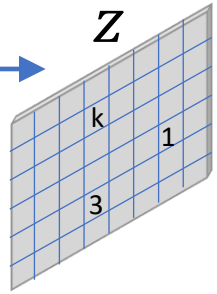
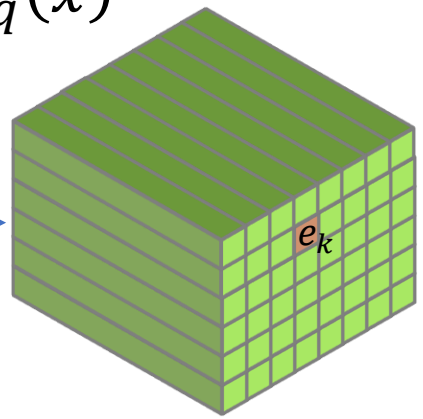




Nearest neighbours index grid

$z_q(x)$



Decoder (CNN)

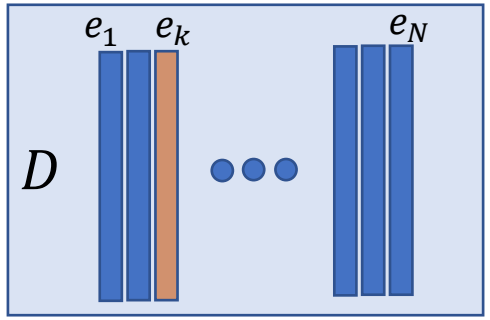
$\hat{x}$

$$q(z=k|x)=\begin{cases}1 & \text{for } \mathrm{k}=\mathrm{argmin}_j\|z_e(x)-e_j\|_2,\\ 0 & \text{otherwise}\end{cases}$$

$$z_q(x)=\mathrm{e_k} \text{ where } \mathrm{k}=\mathrm{argmin_j}\left\|z_e(x)-e_j\right\|^2$$

den Oord et. al, “Neural Discrete Representation Learning”, Neurips’17

Vector Quantize VAE (VQ-VAE)



Codebook (N latent codes)

x

Encoder (CNN)

$z_e(x)$

D

∇L_{z_q}

$z_q(x)$

z

k

3

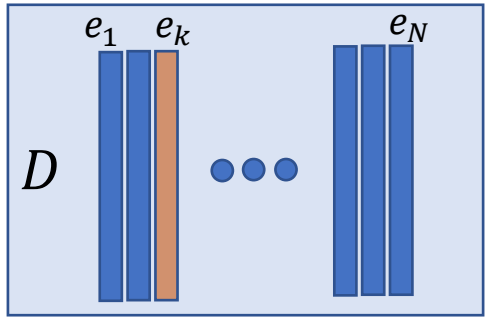
e_k

$\hat{x}$

$$L = \boxed{\log p(x|z_q(x))} + \|\text{sg}[z_e(x)] - e\|_2^2 + \beta\|z_e(x) - \text{sg}[e]\|_2^2,$$

Reconstruction Loss

Vector Quantize VAE (VQ-VAE)

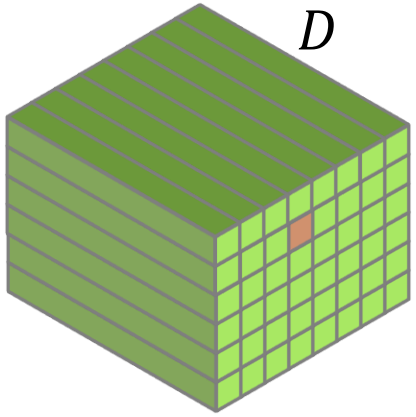


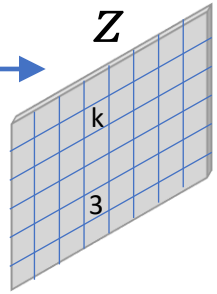
Codebook (N latent codes)

x

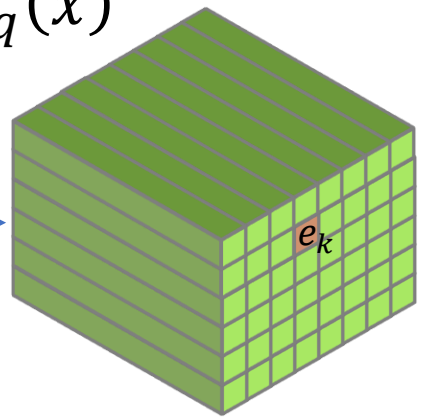
Encoder (CNN)

$z_e(x)$





$z_q(x)$

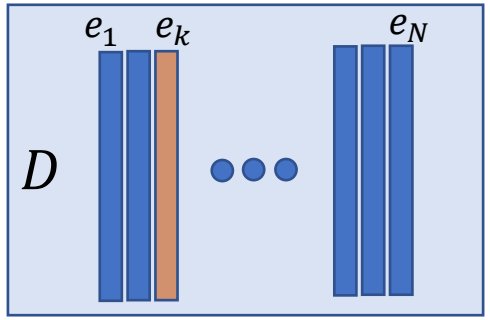


$\hat{x}$

$$L = \log p(x|z_q(x)) + \boxed{\|\text{sg}[z_e(x)] - e\|_2^2} + \beta\|z_e(x) - \text{sg}[e]\|_2^2,$$

codebook alignment

Vector Quantize VAE (VQ-VAE)

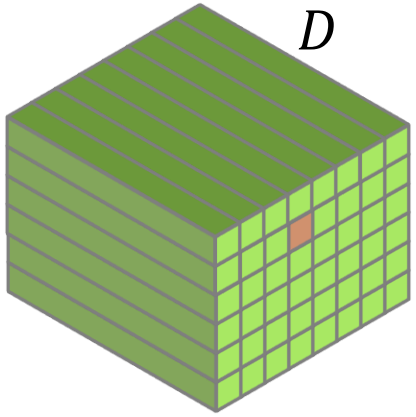


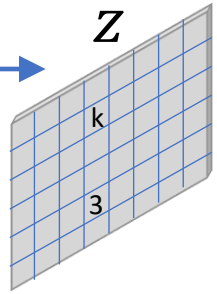
Codebook (N latent codes)

x

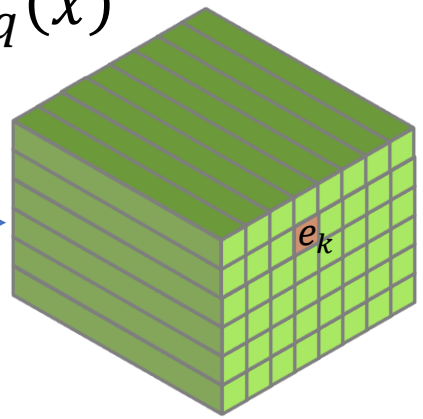
Encoder (CNN)

$z_e(x)$





$z_q(x)$

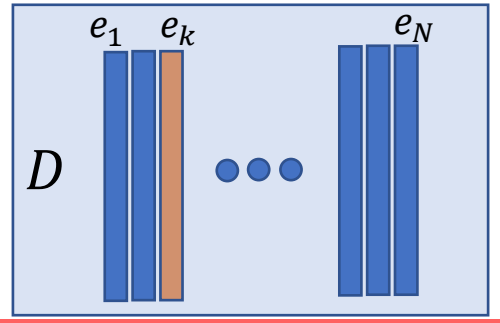


$\hat{x}$

$$L = \log p(x|z_q(x)) + \|\text{sg}[z_e(x)] - e\|_2^2 + \beta \boxed{\|z_e(x) - \text{sg}[e]\|_2^2},$$

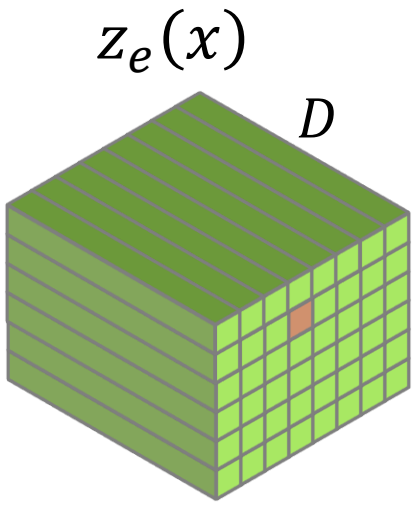
commitment loss

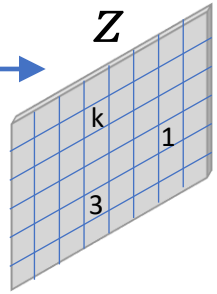
Vector Quantize VAE (VQ-VAE)

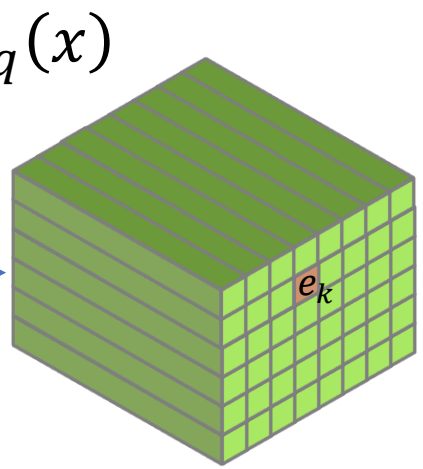


Codebook (N latent codes)

Encoder (CNN)







Decoder (CNN)

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den Oord et. al, “Neural Discrete Representation Learning”, Neurips’17

VQ-VAE Recostruction

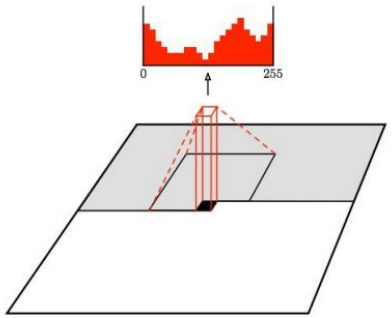
Figure 2: Left: ImageNet 128x128x3 images, right: reconstructions from a VQ-VAE with a 32x32x1 latent space, with K=512.

den Oord et. al, “Neural Discrete Representation Learning”, Neurips’17

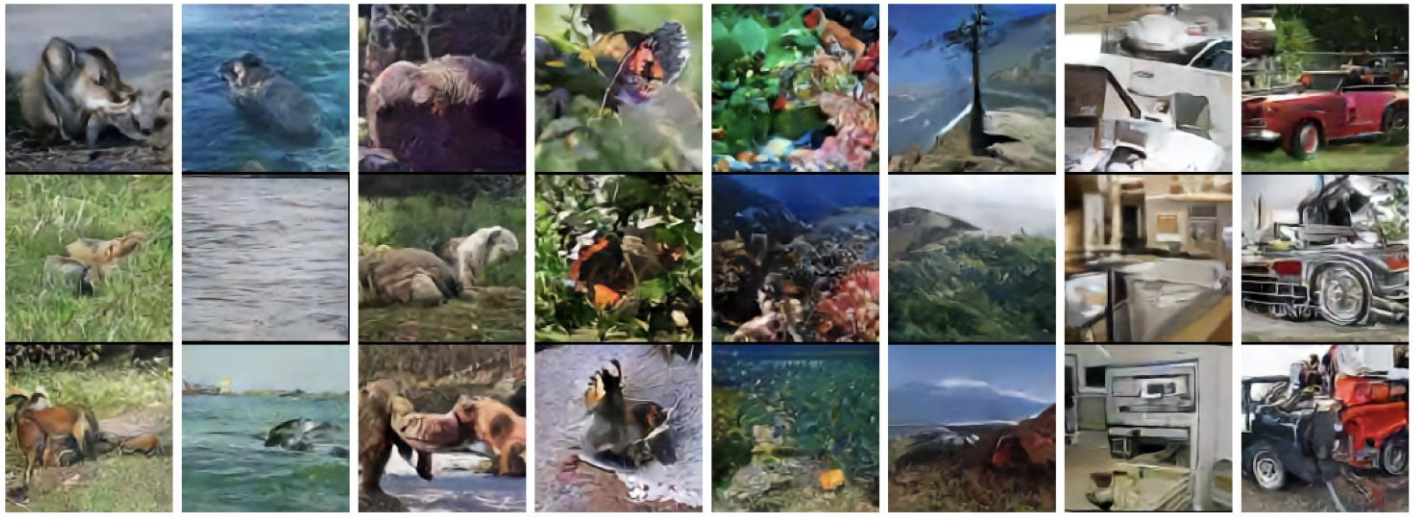
VQ-VAE + PixelCNN

After training, fit an autoregressive distribution over z

$$p_\theta(x) = \prod_{i=1}^{n} p_\theta(x_i | x_1, \ldots, x_{i-1}) \quad \Rightarrow \quad p_\theta(z) = \prod_{i=1}^{n} p_\theta(z_i | z_1, \ldots z_{i-1})$$



PixelCNN



den Oord et. al, “Neural Discrete Representation Learning”, Neurips’17
Razavi et al, “Generating Diverse High-Fidelity Images with VQ-VAE-2”, Neurips’19

VQ-VAE + PixelCNN

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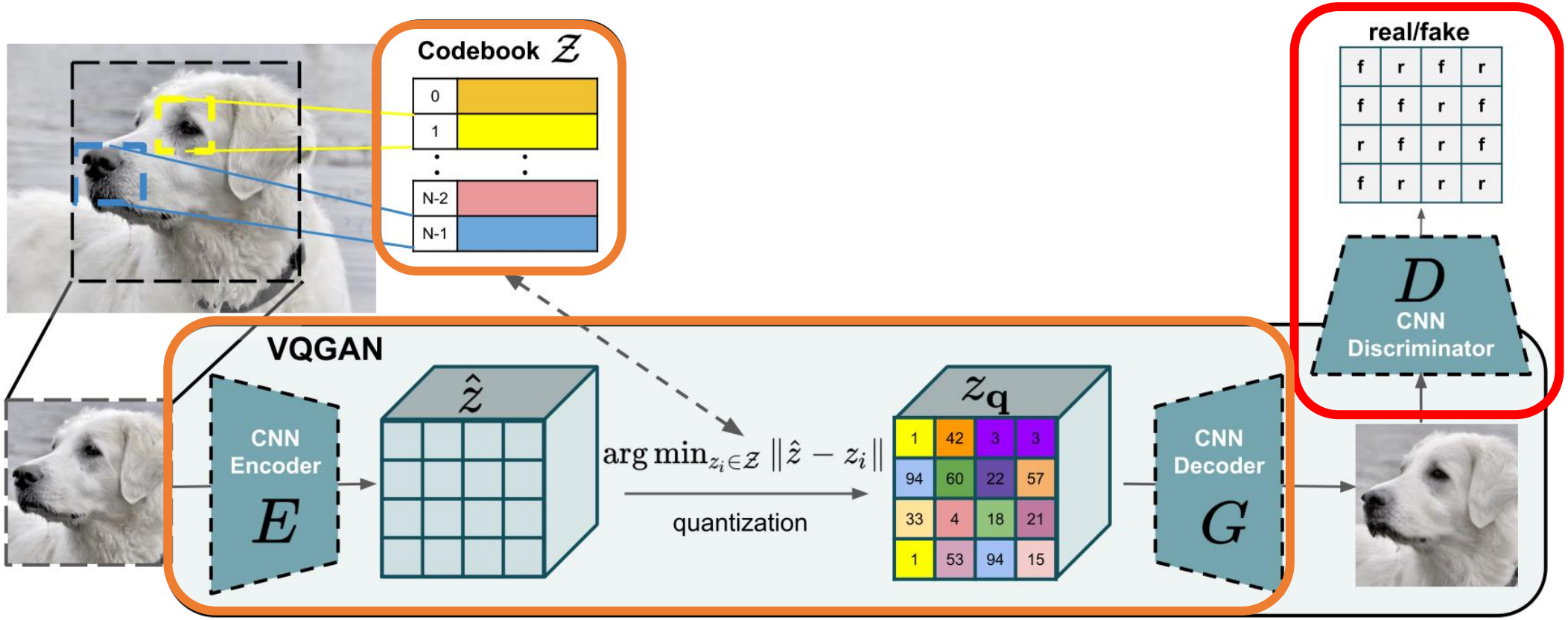
VQ-VAE + GAN (VQ-GAN)

Esser et. al, “Taming Transformers for High-Resolution Image Synthesis”, CVPR’21

VQ-GAN



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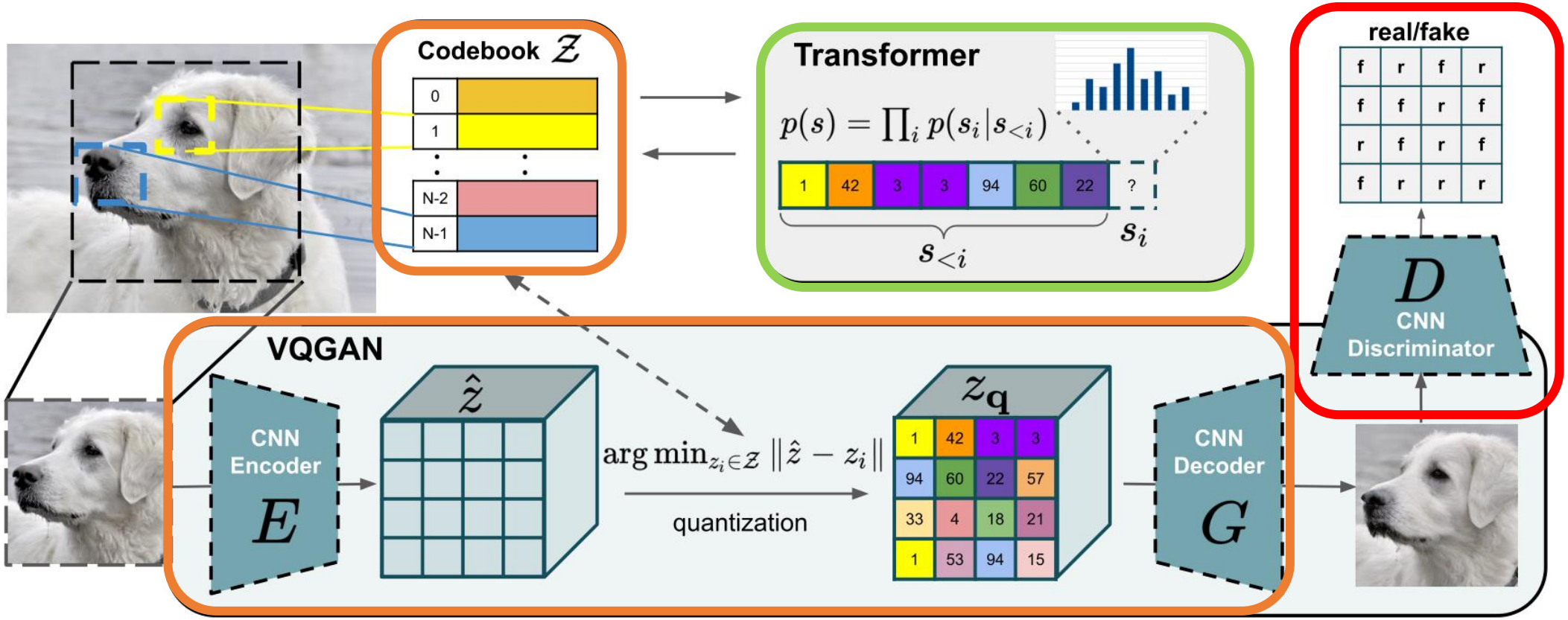
VQ-GAN



VQ-VAE + GAN + Transformer

Esser et. al, “Taming Transformers for High-Resolution Image Synthesis”, CVPR’21

VQ-GAN: CNN+Transformer

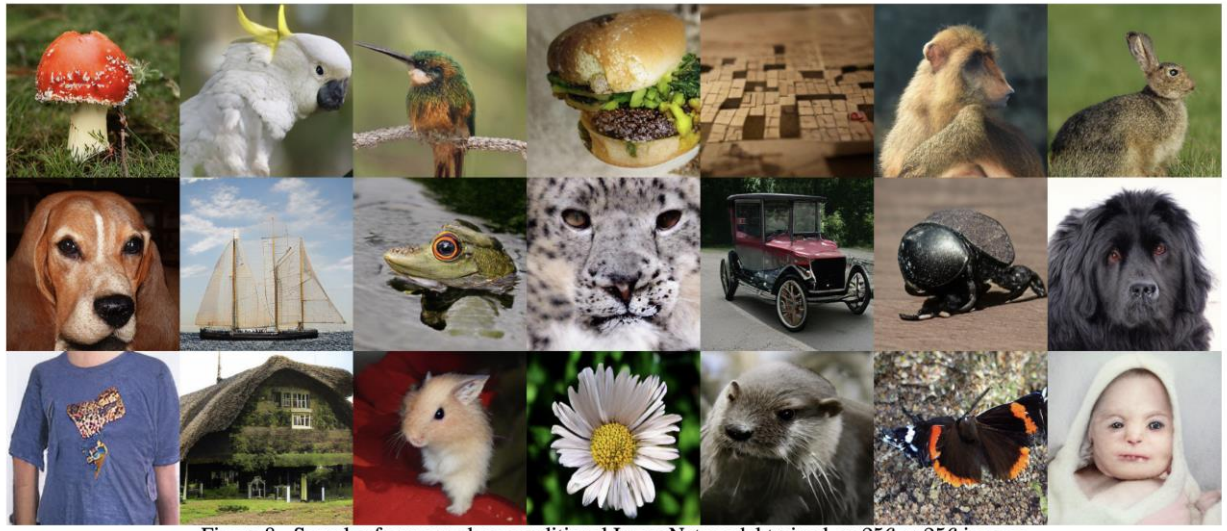
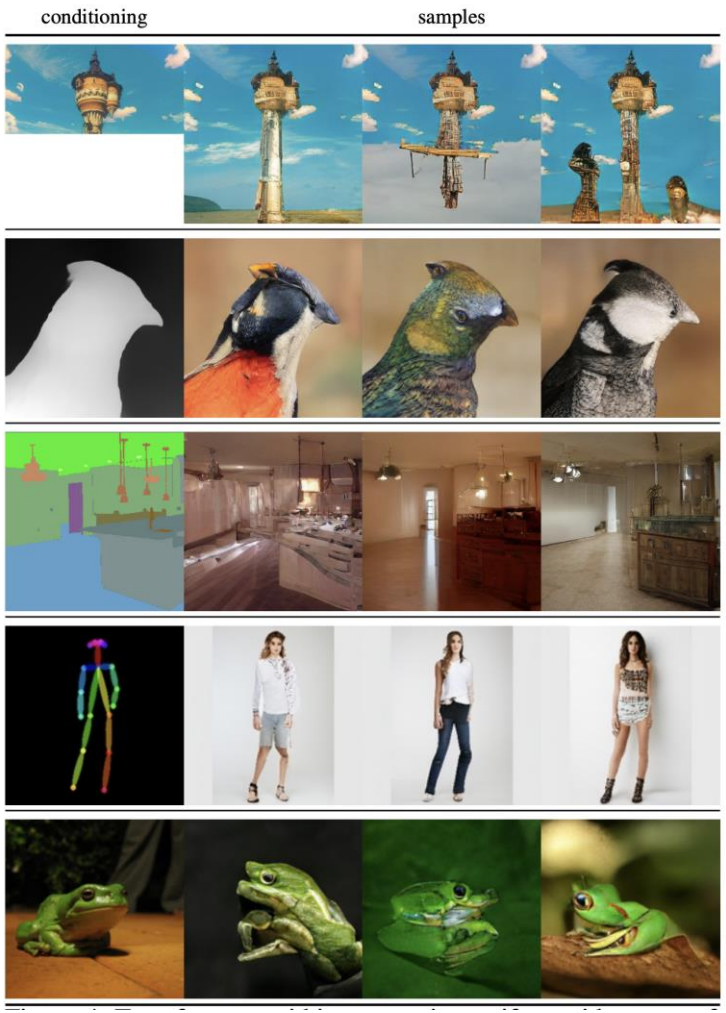


Figure 8. Samples from our class-conditional ImageNet model trained on 256 × 256 images.



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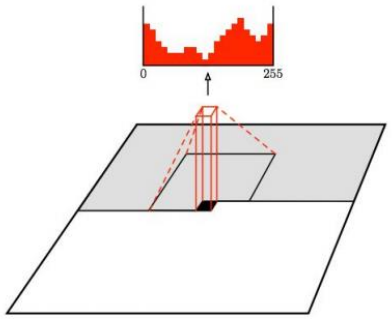
Explicitly density estimation/

Autoregressive image generation



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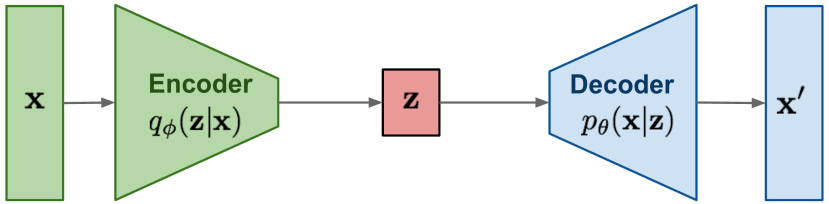
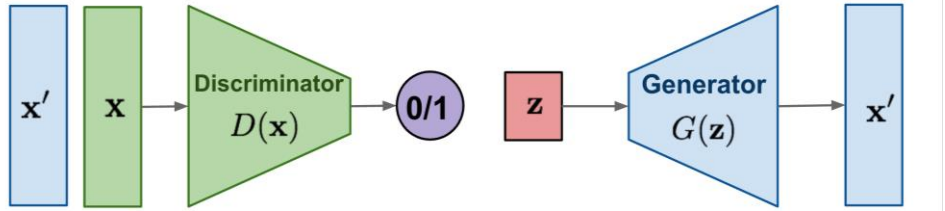


Diffusion Models

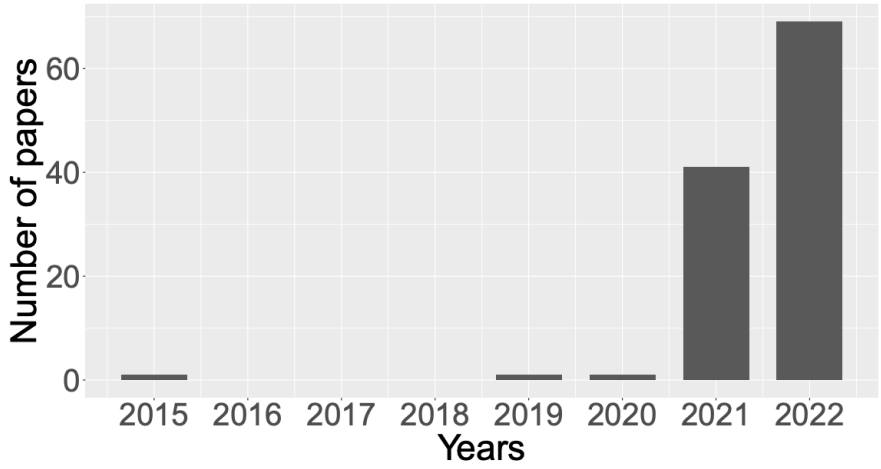
Implicit density estimation

Generative Adversarial Networks (GANs)

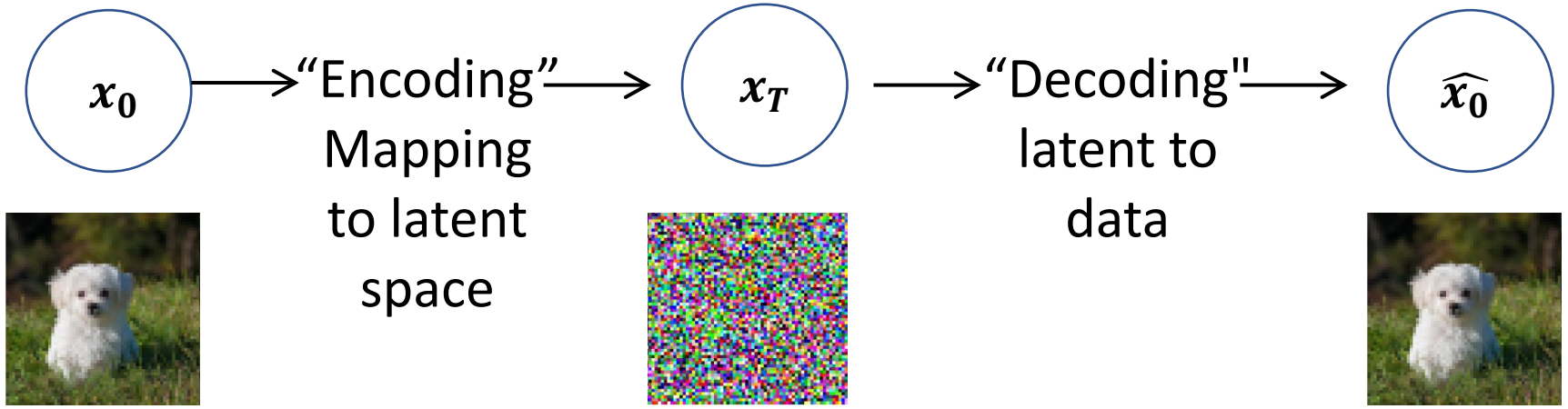


Motivation

Imagen (Google) / DALLE-2 / StableDiffusion

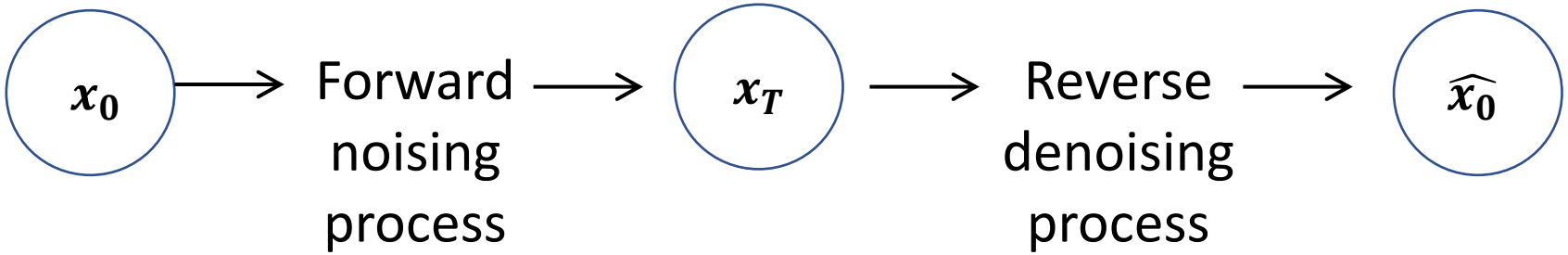


Diffusion Models - Basics

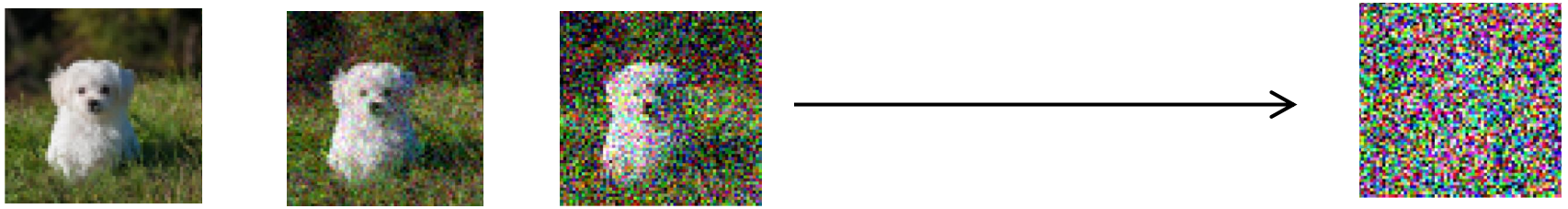


Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein et al. ICML 2015

Diffusion Models - Basics



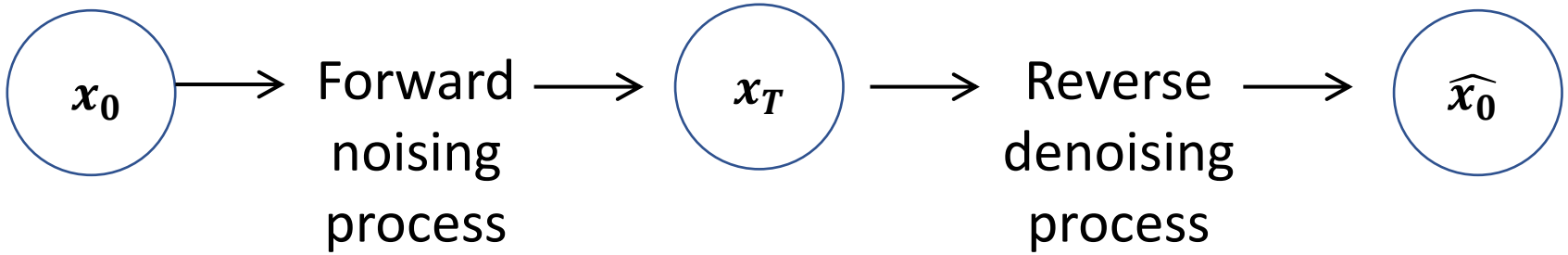
Forward nosing process



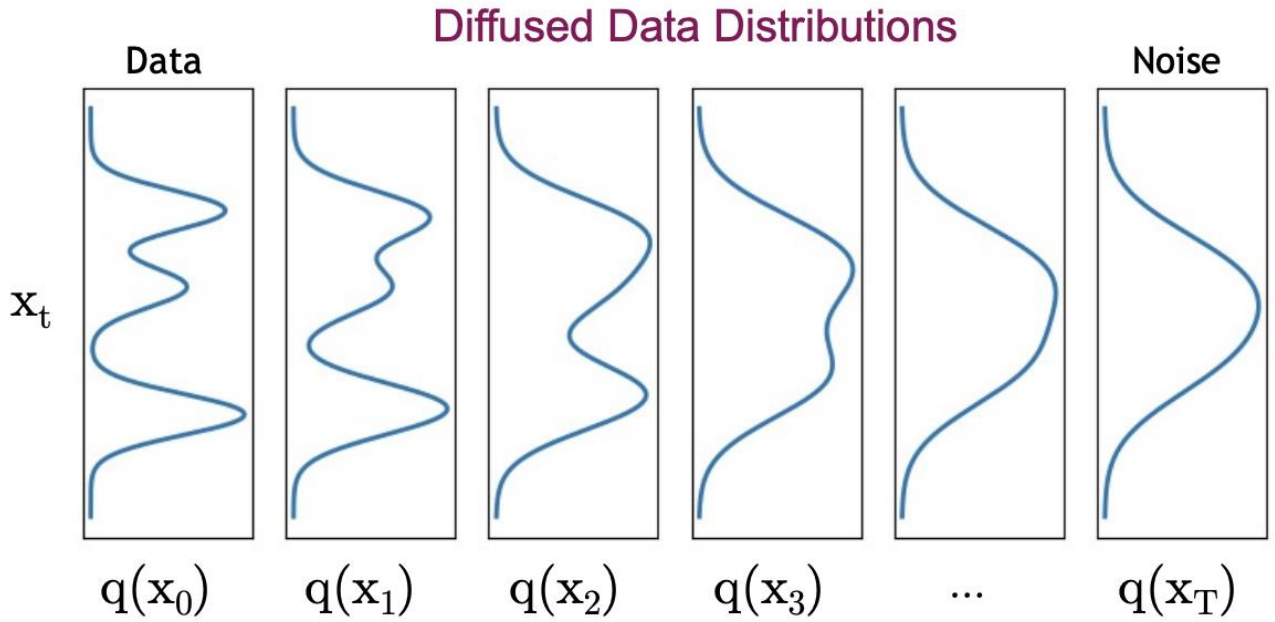
Destructing data by gradually adding noise

"Deep Unsupervised Learning using Nonequilibrium Thermodynamics", Sohl-Dickstein et al. ICML 2015

Diffusion Models - Basics

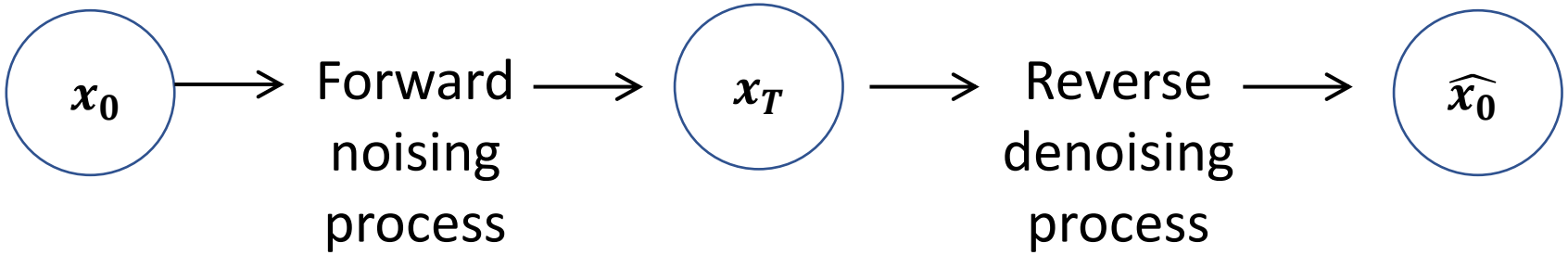


Forward noising process

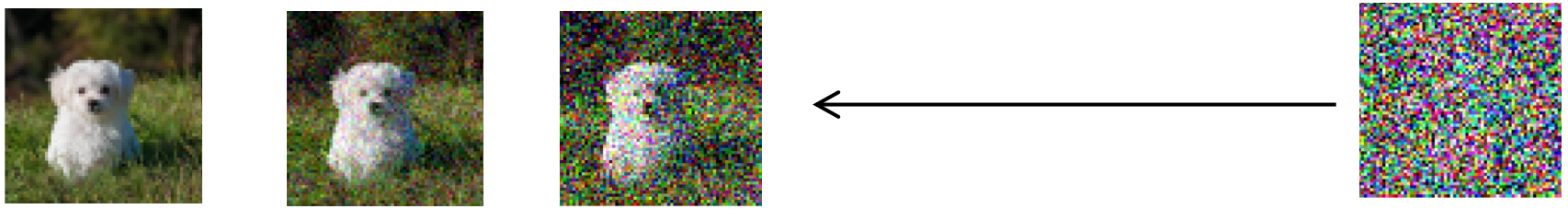


Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein et al. ICML 2015

Diffusion Models - Basics



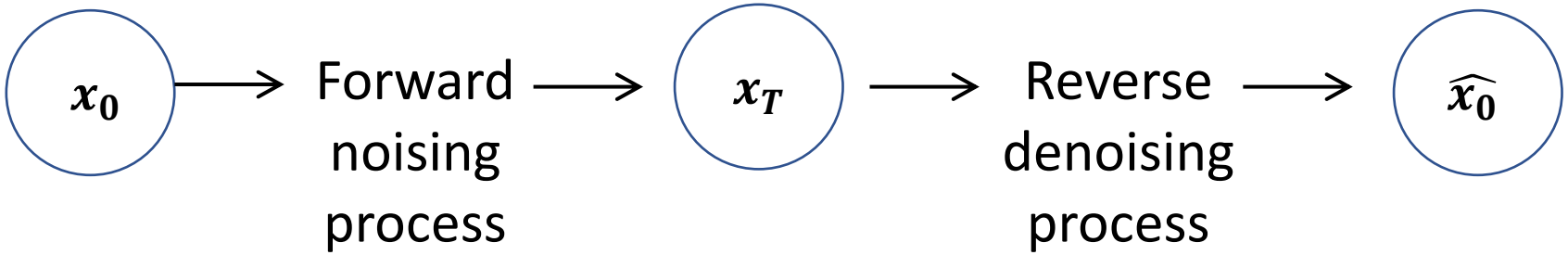
Reverse denoising process

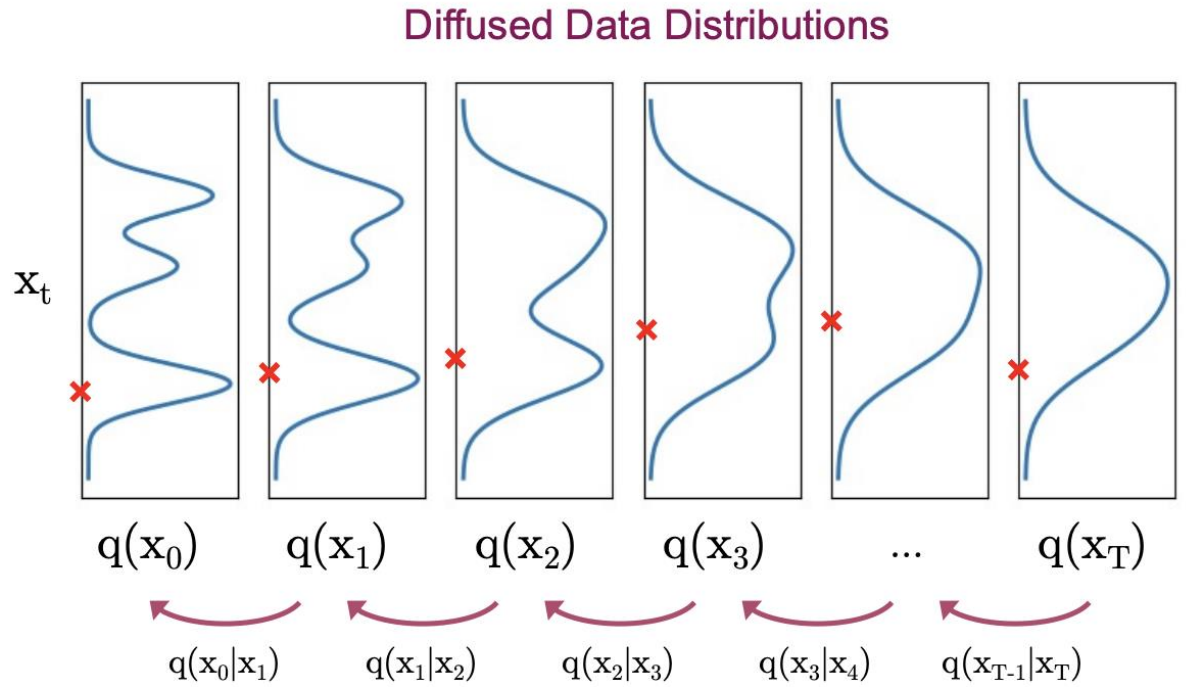


Generating samples by by gradually reducing noise

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein et al. ICML 2015

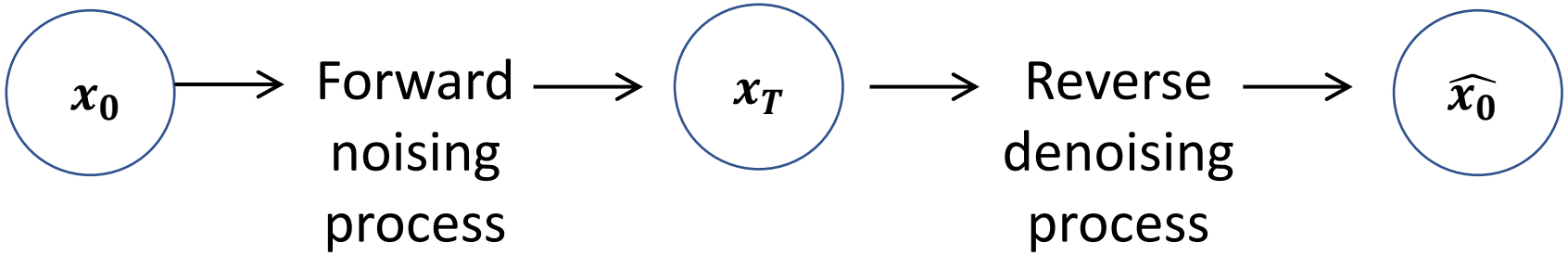
Diffusion Models - Basics





https://cvpr2022-tutorial-diffusion-models.github.io/

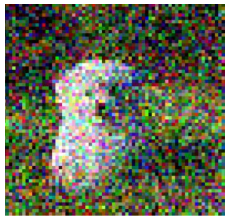
Diffusion Models - Basics



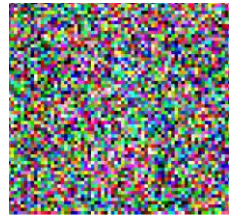
Forward nosing process


x_0


x_1

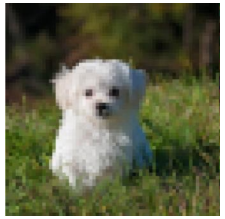


EASY! (and fixed)

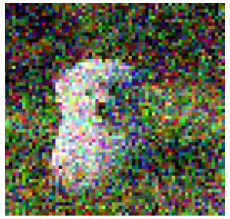

x_T

Destructing data by gradually adding noise

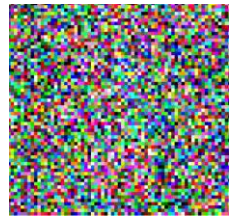
Reverse denosing process


x_0


x_1



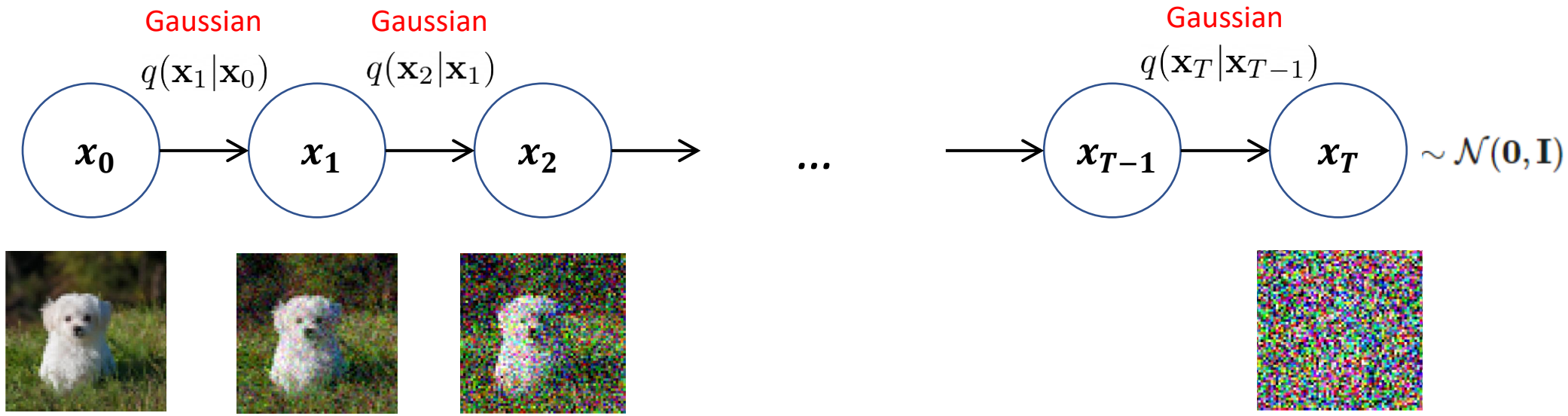
?? NEED A PRIOR ABOUT THE WORLD


x_T

Generating samples by gradually reducing noise

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein et al. ICML 2015

Forward diffusion process



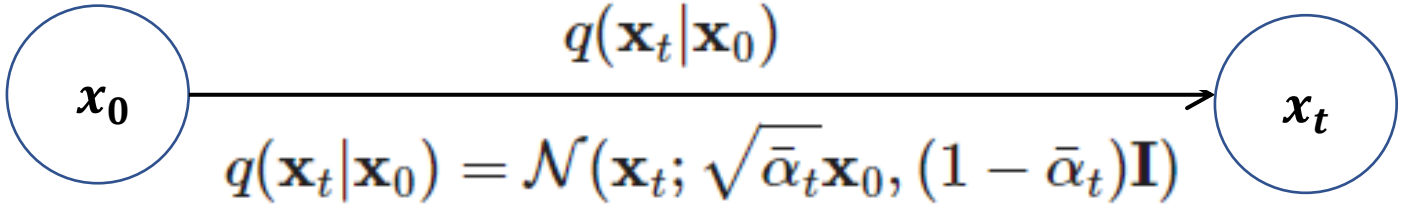
$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$

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

$\beta_t \in (0,1)$

noise schedule
(how much noise to add on step t)

Forward diffusion process: x_t in one step



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

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

Noise scheduling:
Set $\{\beta_t\}$ $s.t., \bar{\alpha}_T \to 0$ and $q(x_T|x_0) \approx \mathcal{N}(x_T; 0, \mathrm{I})$
$\beta_1 < \beta_2 \ldots < \beta_T$

Define $\alpha_t = 1 - \beta_t$:

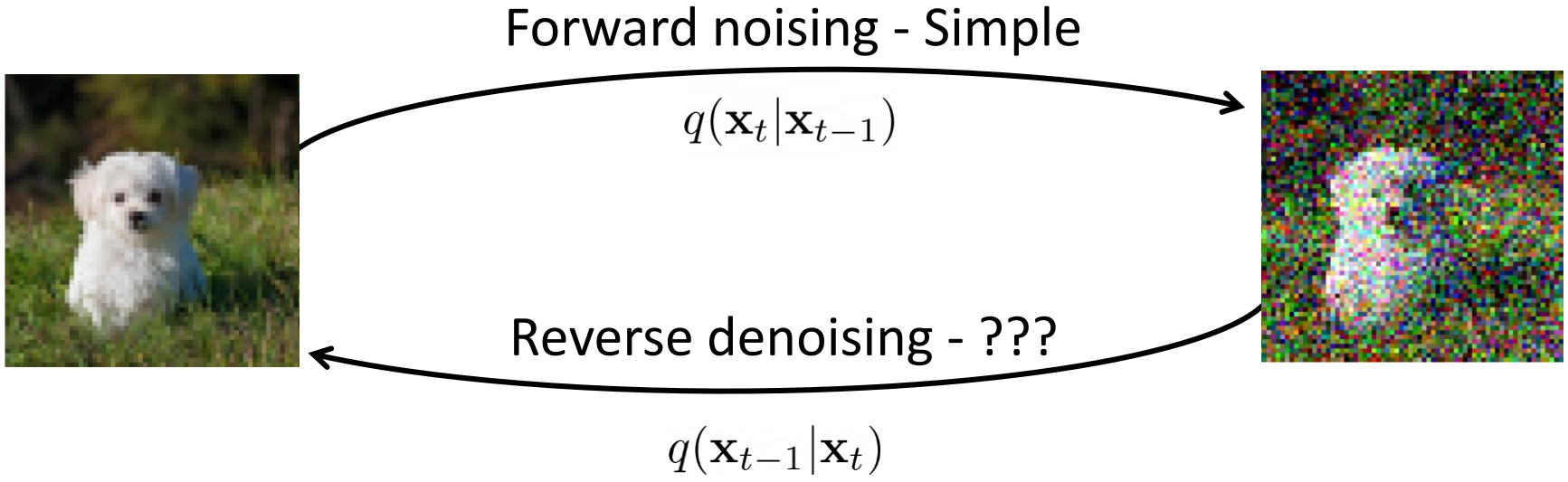
Reparameterization trick:

$$\mathbf{x}_t = \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\mathbf{z}_{t-1} \qquad \mathbf{z}_{t-1} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \qquad \bar{\alpha}_t = \prod_{i=1}^{T} \alpha_i$$

$$= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \underbrace{\sqrt{\alpha_t(1-\alpha_{t-1})}\mathbf{z}_{t-2} + \sqrt{1-\alpha_t}\mathbf{z}_{t-1}}_{\sqrt{1-\alpha_t\alpha_{t-1}}\bar{\mathbf{z}}_{t-2}}$$

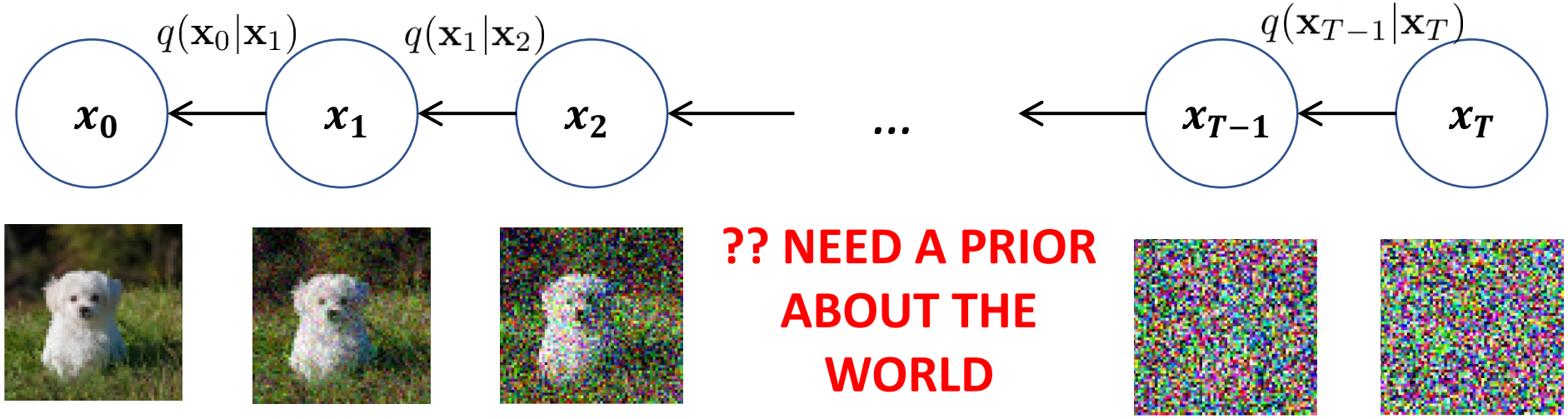
$$= \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\mathbf{z}$$

Reverse diffusion process



Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein et al. ICML 2015

Reverse diffusion process



Generation: sample x_T and iteratively sample:

$x_{t-1} \sim q(x_{t-1}|x_t)$

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

Intractable

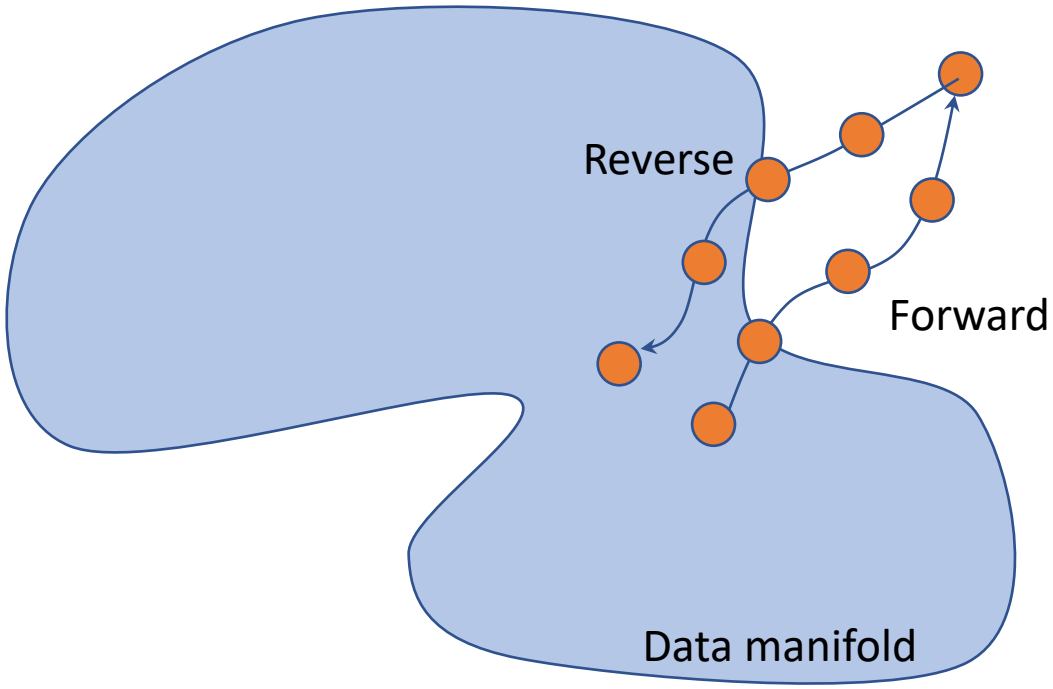
Can we approximate $q(x_{t-1}|x_t)$?

Yes! if $\beta_t \ll 1$ – small variance in each forward step

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_t^2 \mathbf{I})$$

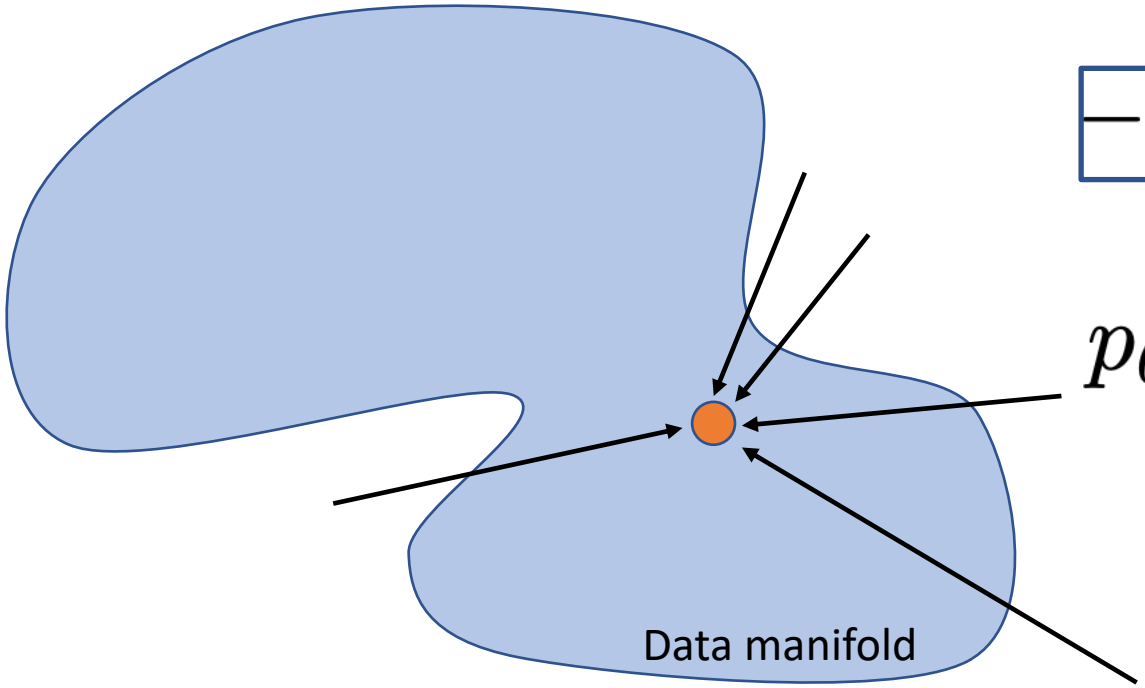
Train a network to predict the reverse distribution

Forward and Reverse Diffusion



Objective?

Ideally: maximize the likelihood of the data after reverse process, i.e., minimize:



$$-\mathbb{E}_{q(x_0)} \log p_\theta(x_0)$$

$$p_\theta(x_0) = \int p_\theta(x_{0:T}) dx_{1:T}$$

$$\mathbb{E}_{q(x_0)} \log p_\theta(x_0) \geq variational\ lower\ bound$$

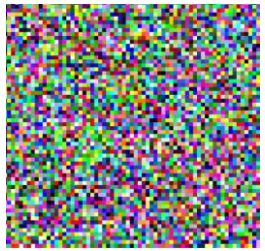
$$-\mathbb{E}_{q(x_0)} \log p_\theta(x_0) \leq variational\ upper\ bound$$

Training

Sample $\mathbf{x}_0$ from the training set

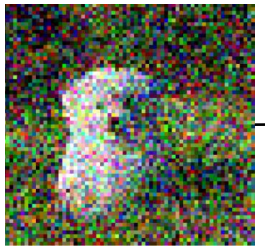
Sample timestep $t \sim U(1, T)$

Sample noise $\mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$



(Forward process)

Calculate $\mathbf{x}_t$ using sampled noise



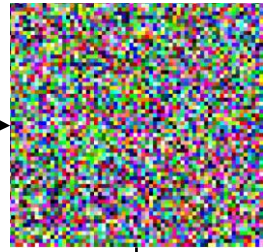
Reminder:

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\,\mathbf{z}_t$$

Neural Net

(Reverse process)

Predict $\mathbf{z}_\theta$



Take gradient step on

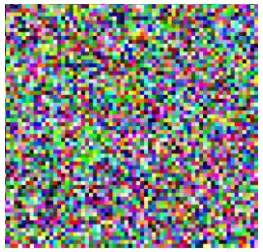
$$\nabla_\theta \left\| \mathbf{z}_t - \mathbf{z}_\theta \left(\mathbf{x}_t, t \right) \right\|^2$$

Denoising Diffusion Probabilistic Models, Ho et al. NeurIPS 2020

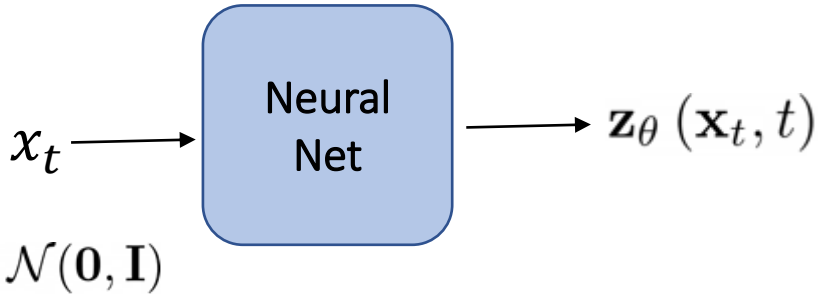
Sampling Algorithm

Reminder: $p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_t^2 \mathbf{I})$

1. Sample $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$



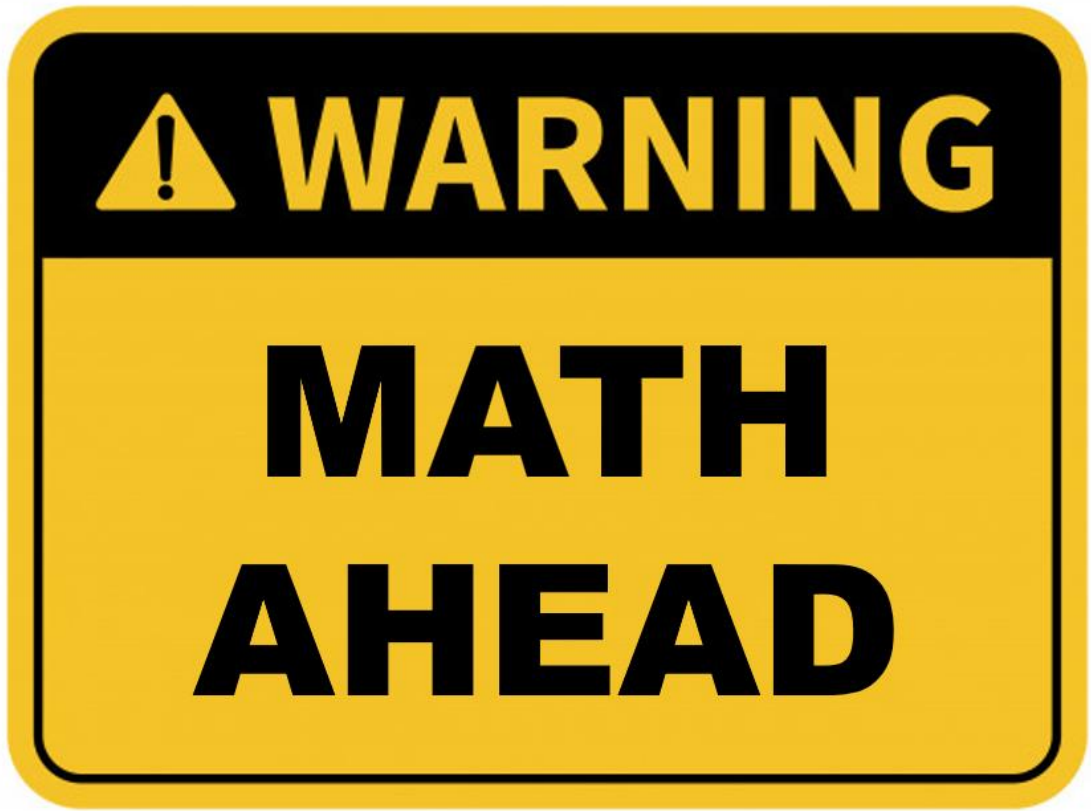
2. For $t = T, \ldots, 1$:
   - "Predict noise" in x_t
   - Sample variance noise $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
   - Sample from reverse distribution:



$$x_{t-1} = \mu_\theta(z_\theta, x_t, t) + \sigma_t^2 z$$

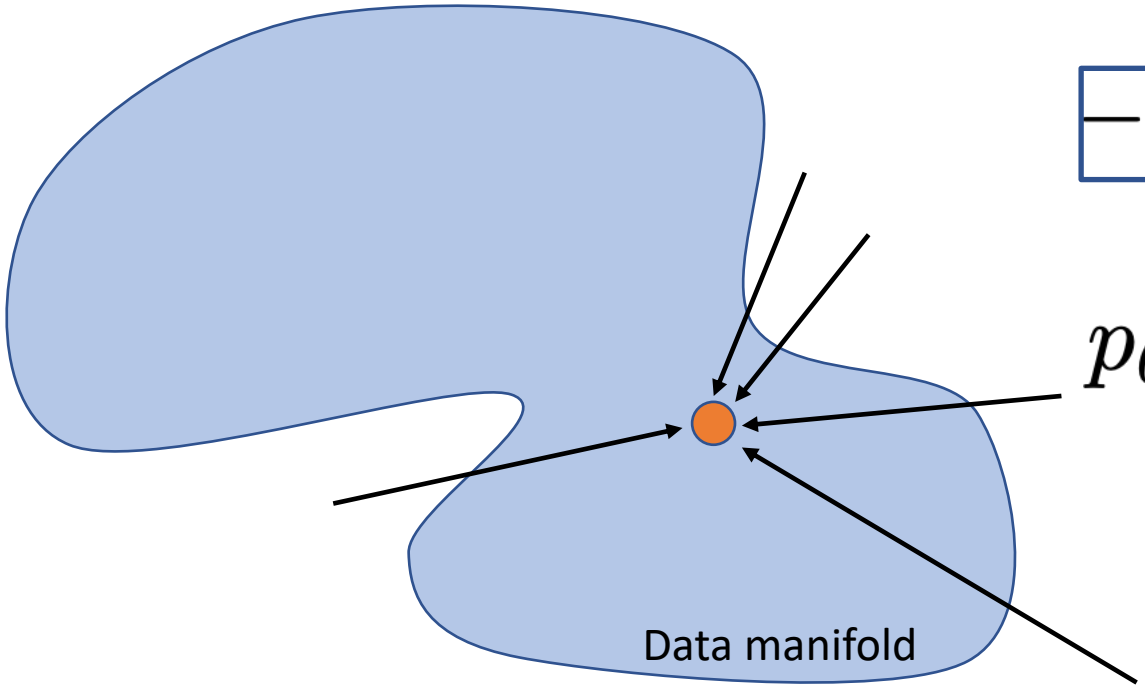
3. Return

Denoising Diffusion Probabilistic Models, Ho et al. NeurIPS 2020


WARNING
MATH
AHEAD

Objective?

Ideally: maximize the likelihood of the data after reverse process, i.e., minimize:



$$-\mathbb{E}_{q(x_0)} \log p_\theta(x_0)$$

$$p_\theta(x_0) = \int p_\theta(x_{0:T}) dx_{1:T}$$

$$\mathbb{E}_{q(x_0)} \log p_\theta(x_0) \geq variational\ lower\ bound$$

$$-\mathbb{E}_{q(x_0)} \log p_\theta(x_0) \leq variational\ upper\ bound$$

ELBO Objective

x – observation
z – latent

$$\log p_\theta(x) \geq \underbrace{\mathbb{E}_{q(z|x)} \log p_\theta(x|z)}_{\text{Reconstruction term}} - \underbrace{D_{KL}(q(z|x) \,||\, p_\theta(z))}_{\text{Latent prior term}}$$

x_0 – observation
$x_{1:T}$ – latent

Objective

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

$$-\mathbb{E}_{q(x_0)} \log p_\theta(x_0) \leq \mathbb{E}_q \left[\log \frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)} \right]$$

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

Full derivation: Appendix B in Sohl-Dickstein et al. 2015

Objective

$$-\mathbb{E}_{q(x_0)} \log p_\theta(x_0) \leq \mathbb{E}_q \left[\log \frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)} \right] = \mathbb{E}_q \left[\log x_T \right] + \sum_{t \geq 1} \log \frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})} := L_{VLB}$$

$$L_{VLB} = \mathbb{E}_q \left[\underbrace{-D_{KL}(q(x_T|x_0)||p(x_T))}_{\text{Prior matching}} - \sum_{t>1} D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) + \log p_\theta(x_0|x_1) \right]$$

Final noised input

Gaussian (fixed)

Full derivation: Appendix B in Sohl-Dickstein et al. 2015

Objective

$$-\mathbb{E}_{q(x_0)} \log p_\theta(x_0) \leq \mathbb{E}_q \left[\log \frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)} \right] = \mathbb{E}_q \left[\log x_T \right] + \sum_{t \geq 1} \log \frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})} := L_{VLB}$$

$$L_{VLB} = \mathbb{E}_q \left[\underbrace{-D_{KL}(q(x_T|x_0)||p(x_T))}_{\text{Prior matching}} - \sum_{t>1} D_{KL}(\underbrace{q(x_{t-1}|x_t, x_0)}_{\text{Gaussian}} || \underbrace{p_\theta(x_{t-1}|x_t)}_{\text{Gaussian}}) + \underbrace{\log p_\theta(x_0|x_1)}_{\text{Reconstruction term}} \right]$$

Final noised input

Gaussian (fixed)

Denoising matching

x_t x_0 x_{t-1}

Closed form!

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

Denoising Diffusion Probabilistic Models, Ho et al. NeurIPS 2020

$$L_{VLB} = -\mathbb{E}_{q,t}[D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))]$$

x_t x_0 x_{t-1}

$$q(x_{t-1}|x_t, x_0) := \mathcal{N}(x_{t-1};\ \tilde{\mu}_t(x_t, x_0), \tilde{\beta}_t \boldsymbol{I})$$

$$p_\theta(x_{t-1}|x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_t^2 \boldsymbol{I})$$

Learnable Fixed

Ground truth vs. predicted reverse process

Unspervised learning → Regression:

$$L_{t-1} = D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)$$
$$= \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\|\tilde{\mu}_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2\right] + C$$

DDPM, Ho et al. NeurIPS 2020:

$$\tilde{\mu}_t(x_t, x_0) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right). \qquad \epsilon \sim \mathcal{N}(0,1)$$
$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$$

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

Use a noise prediction network: $L_{t-1} = \mathbb{E}_{x_0,\epsilon}[\lambda_t\|\epsilon - \epsilon_\theta(x_t, t)\|^2] + C$

$$L_{simple} = \mathbb{E}_{x_0\sim q(x_0),\epsilon\sim\mathcal{N}(0,I),t\sim U(1,T)}[\|\epsilon - \epsilon_\theta(x_t, t)\|^2]$$

Summary

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
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

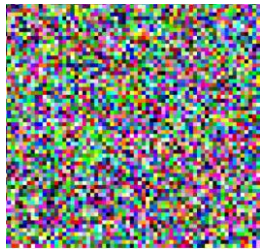
Denoising Diffusion Probabilistic Models, Ho et al. NeurIPS 2020

Training

Sample $\mathbf{x}_0$ from the training set

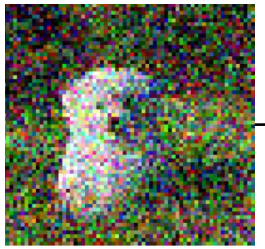
Sample timestep $t \sim U(1, T)$

Sample noise $\mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$



(Forward process)

Calculate $\mathbf{x}_t$ using sampled noise



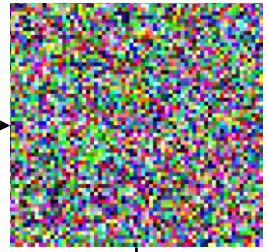
Reminder:

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\,\mathbf{z}_t$$

Neural Net

(Reverse process)

Predict $\mathbf{z}_\theta$



Take gradient step on

$$\nabla_\theta \left\| \mathbf{z}_t - \mathbf{z}_\theta \left(\mathbf{x}_t, t \right) \right\|^2$$

Denoising Diffusion Probabilistic Models, Ho et al. NeurIPS 2020

Summary

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
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

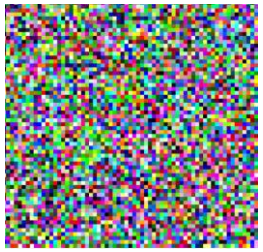
Algorithm 2 Sampling

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** $\mathbf{x}_0$

Denoising Diffusion Probabilistic Models, Ho et al. NeurIPS 2020

Reminder: $p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_t^2 \mathbf{I})$

Sampling Algorithm



Neural Net

1. Sample $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2. For $t = T, \ldots, 1$:
   - "Predict noise" in current image $\mathbf{z}_\theta(\mathbf{x}_t, t)$
   - Sample variance noise $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
   - Sample from reverse distribution:

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

3. Return $\mathbf{x}_0$

Denoising Diffusion Probabilistic Models, Ho et al. NeurIPS 2020

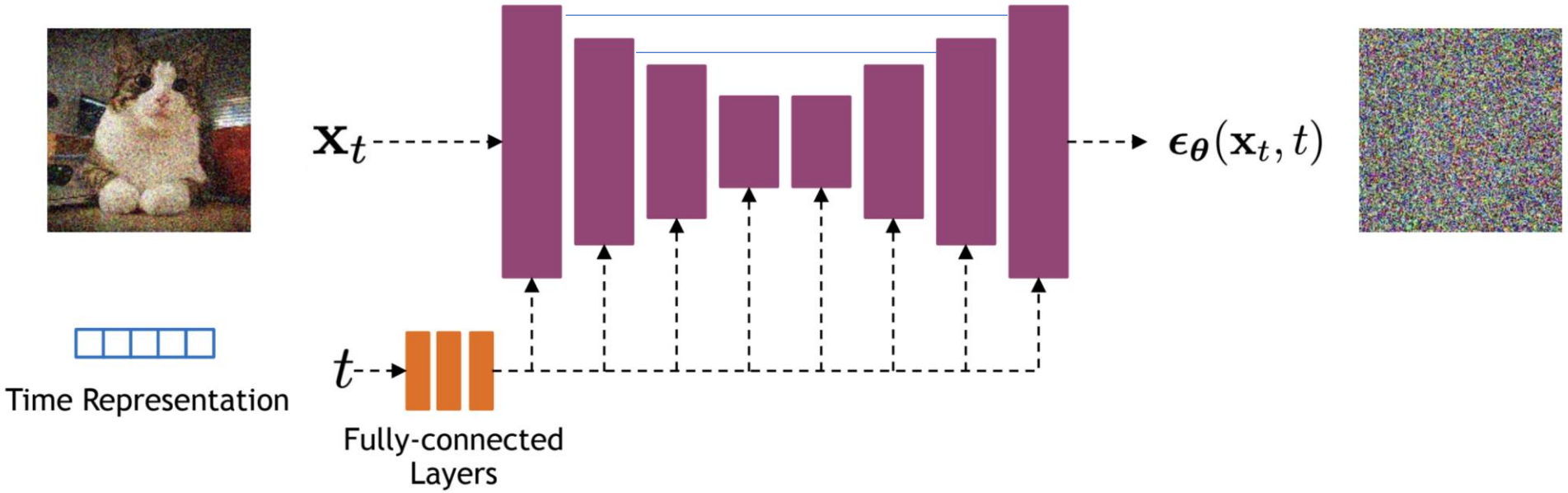
Predicted $\hat{x}$

Recall (reparameterization trick): $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon$

$$\widehat{x}_0 = \frac{x_t}{\sqrt{\bar{\alpha}_t}} - \frac{\sqrt{1 - \bar{\alpha}_t}\epsilon_\theta(x_t, t)}{\sqrt{\bar{\alpha}_t}}$$

Implementation

Often use U-Net architectures with ResNet blocks and self-attention layers



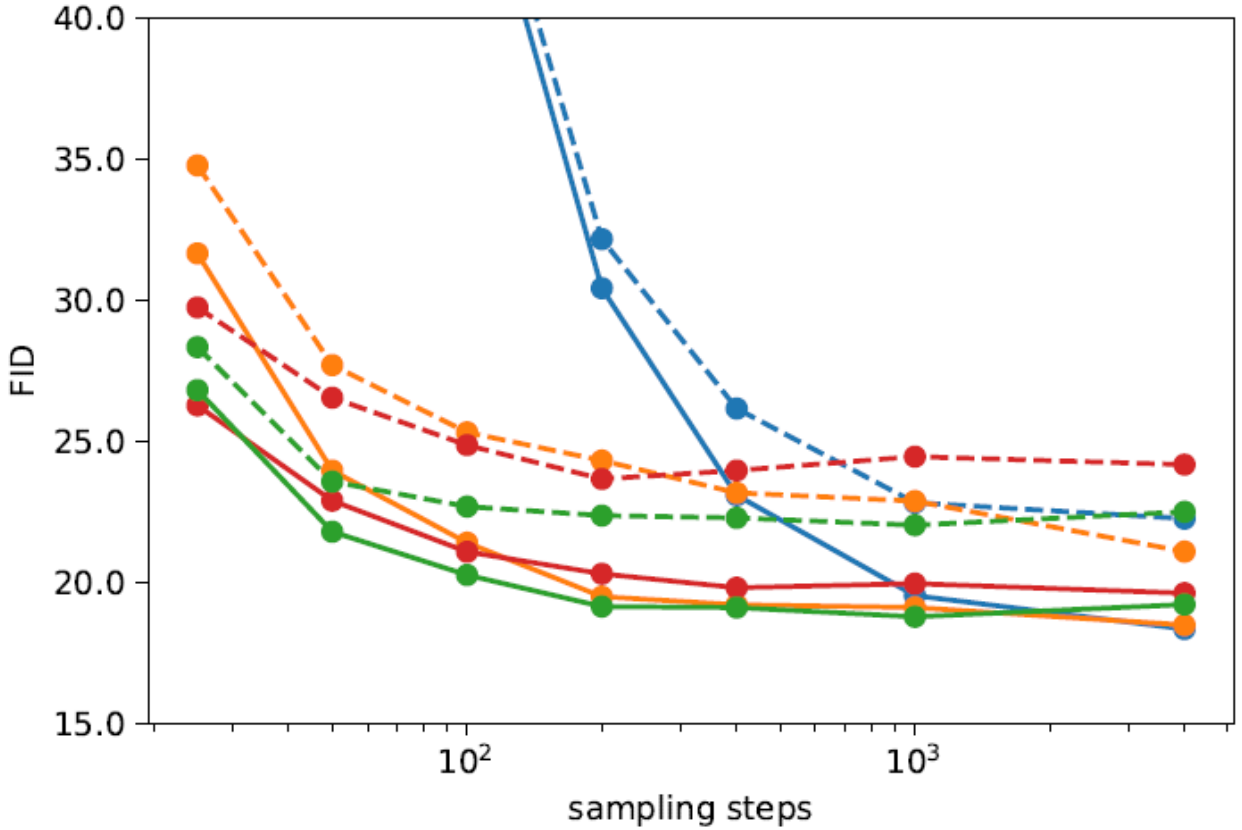
Time features are fed to the residual blocks using either simple spatial addition or using adaptive group normalization layers. (see Dharivwal and Nichol NeurIPS 2021)

Slide credit :[Tutorial on Denoising Diffusion-based Generative Modeling: Foundations and Applications]

Improving sampling speed

Problem: sampling takes too long (several minutes for one 64*64 image)

Solution: Just skip some sampling steps!



Diffusion models beat GANs ?

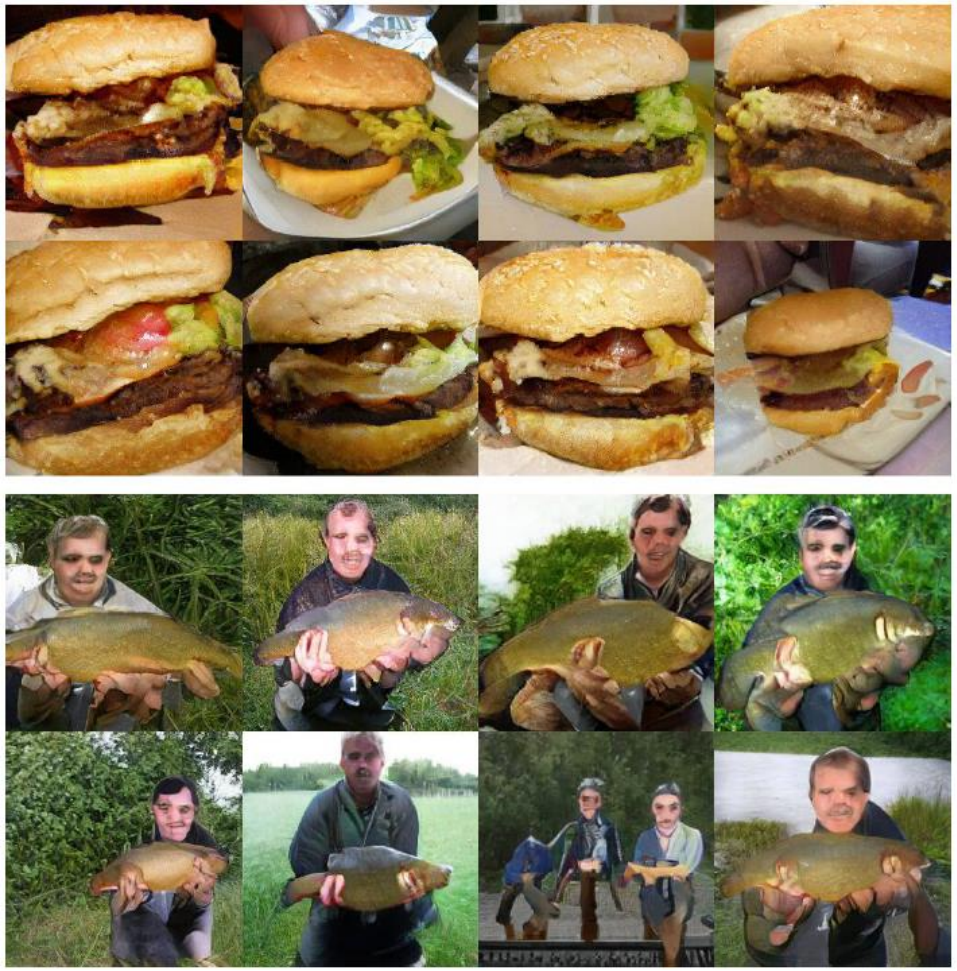
BigGAN

DDPM improved

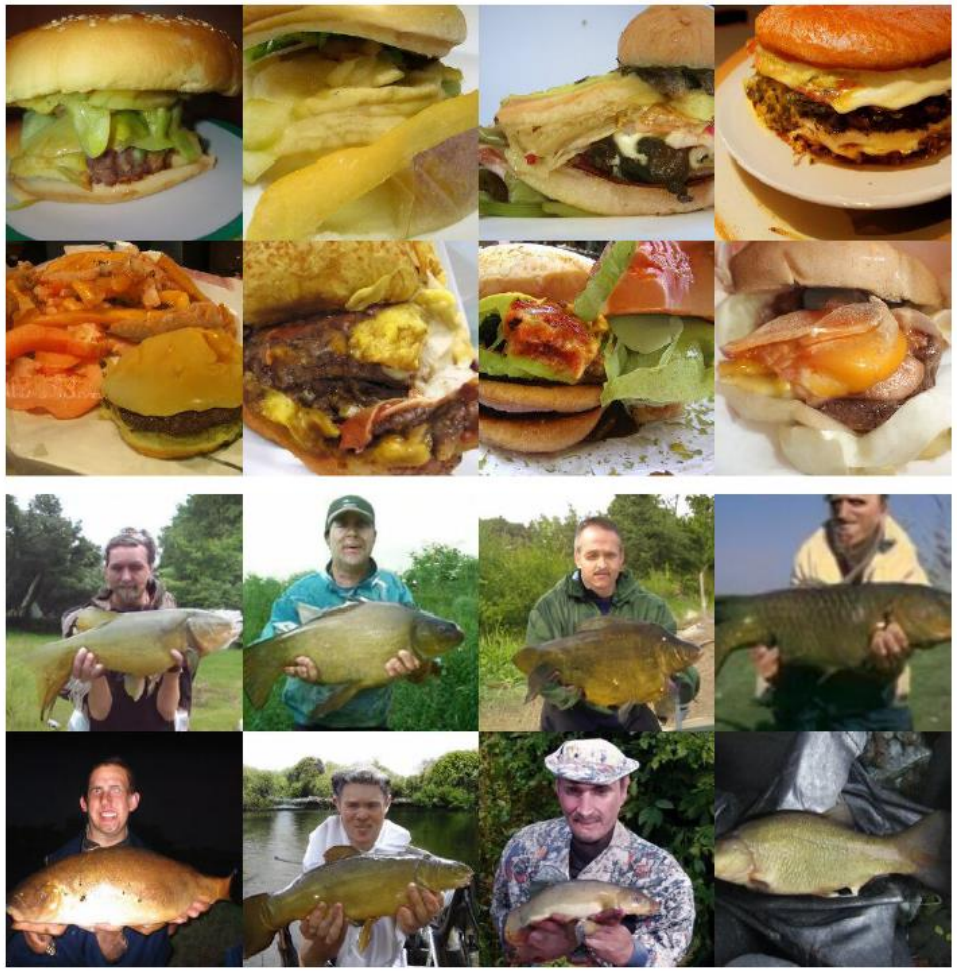
Dhariwal, P. and Nichol, A., 2021. “**Diffusion Models Beat GANs on Image Synthesis**.” arXiv e-prints, pp.arXiv-2105.

Diffusion models beat GANs ?

BigGAN



DDPM improved



Dhariwal, P. and Nichol, A., 2021. “**Diffusion Models Beat GANs on Image Synthesis**.” arXiv e-prints, pp.arXiv-2105.

Conditional Generation

- Class label
- Text
- Another image
- Depth map

$$p_\theta(x_0|y)$$

Let's just input the conditional signal:

$$\epsilon_\theta(x_t, t, y)$$

Image super-resolution: y is a low-resolution image, x is the corresponding high-resolusion image
Training data: a collection of high/low resolution images $\{x_i, y_i\}$

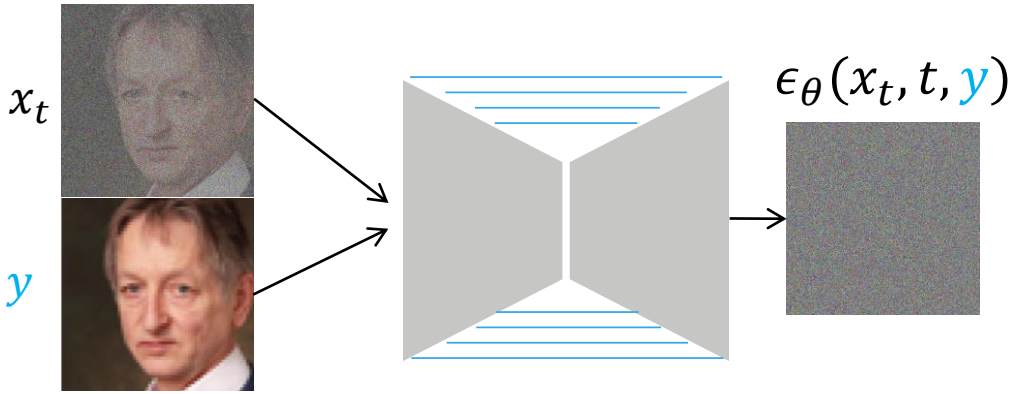
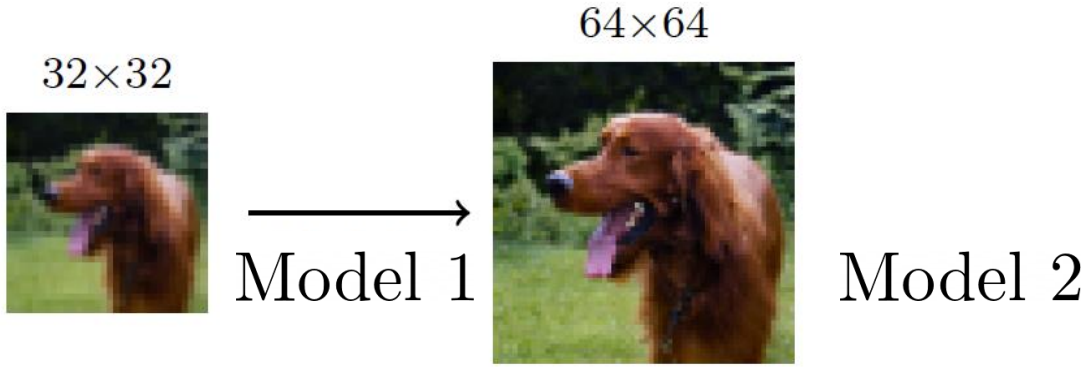


Image Super-Resolution via Iterative Refinement, Saharia et al. 2021

Cascaded Diffusion Models



Stacking diffusion models advantages:

- Smaller models
- Training in parallel
- Individual number of steps tuning

Image Super-Resolution via Iterative Refinement, Saharia et al. 2021

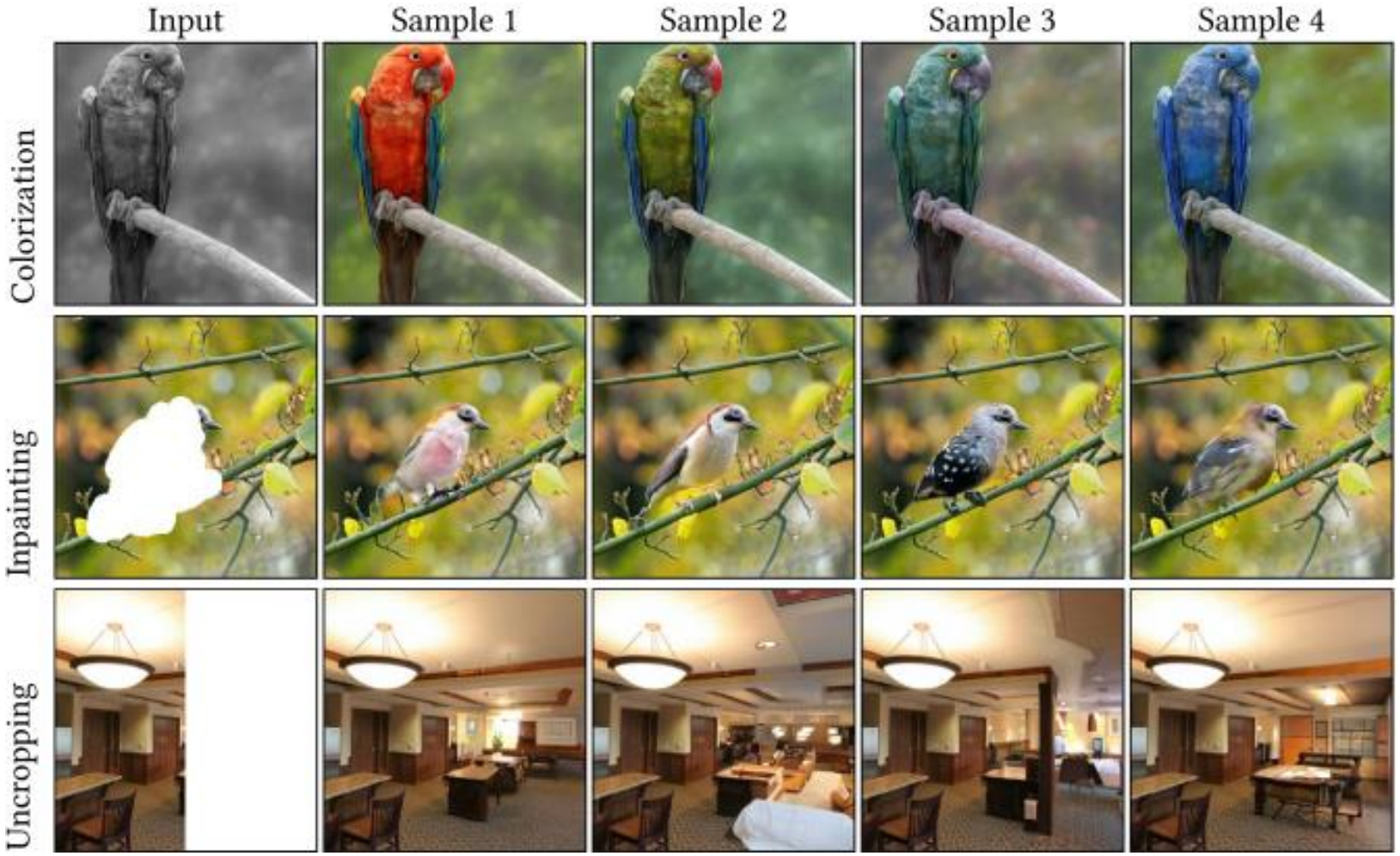
(64×64)

(256×256)

(1024×1024)

Image Super-Resolution via Iterative Refinement, Saharia et al. 2021

Image-to-Image Translation Tasks



Saharia et. al., Palette: Image-to-Image Diffusion Models

Resources:

- [Tutorial on Denoising Diffusion-based Generative Modeling: Foundations and Applications](), **CVPR'22**
- [Understanding Diffusion Models: A Unified Perspective, Calvin Luo, Google Research]()
- [What are Diffusion Models?]() **Ari Seff**
- [https://lilianweng.github.io/lil-log/2021/07/11/diffusion-models.html]()
- Dhariwal, P. and Nichol, A., 2021. "**Diffusion Models Beat GANs on Image Synthesis**." arXiv e-prints, pp.arXiv-2105.
- A. Nichol, P. Dhariwal, A. Ramesh, P. Shyam, P. Mishkin, B. McGrew, I. Sutskever, and M. Chen, **"Glide: Towards photorealistic image generation and editing with text-guided diffusion models,"** arXiv preprint arXiv:2112.10741, 2021.

Credit:

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Rafail Fridman

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Next class/tutorial

Self-supervised learning

Yaniv Nikankin