# CS 4644-DL / 7643-A
# ZSOLT KIRA

Generative Models:

Denoising Diffusion Probabilistic Models (DDPMs)

Slides adapted from those by Danfei Xu

- **Assignment 4 – Generative models**
  - Due **March 30th 11:59pm EST**

- **Projects**
  - Project proposal due **March 14th**

- Meta office hours
  - Wed. 3pm ET on Machine Translation
  - Friday 3pm ET on Embeddings

# Taxonomy of Generative Models

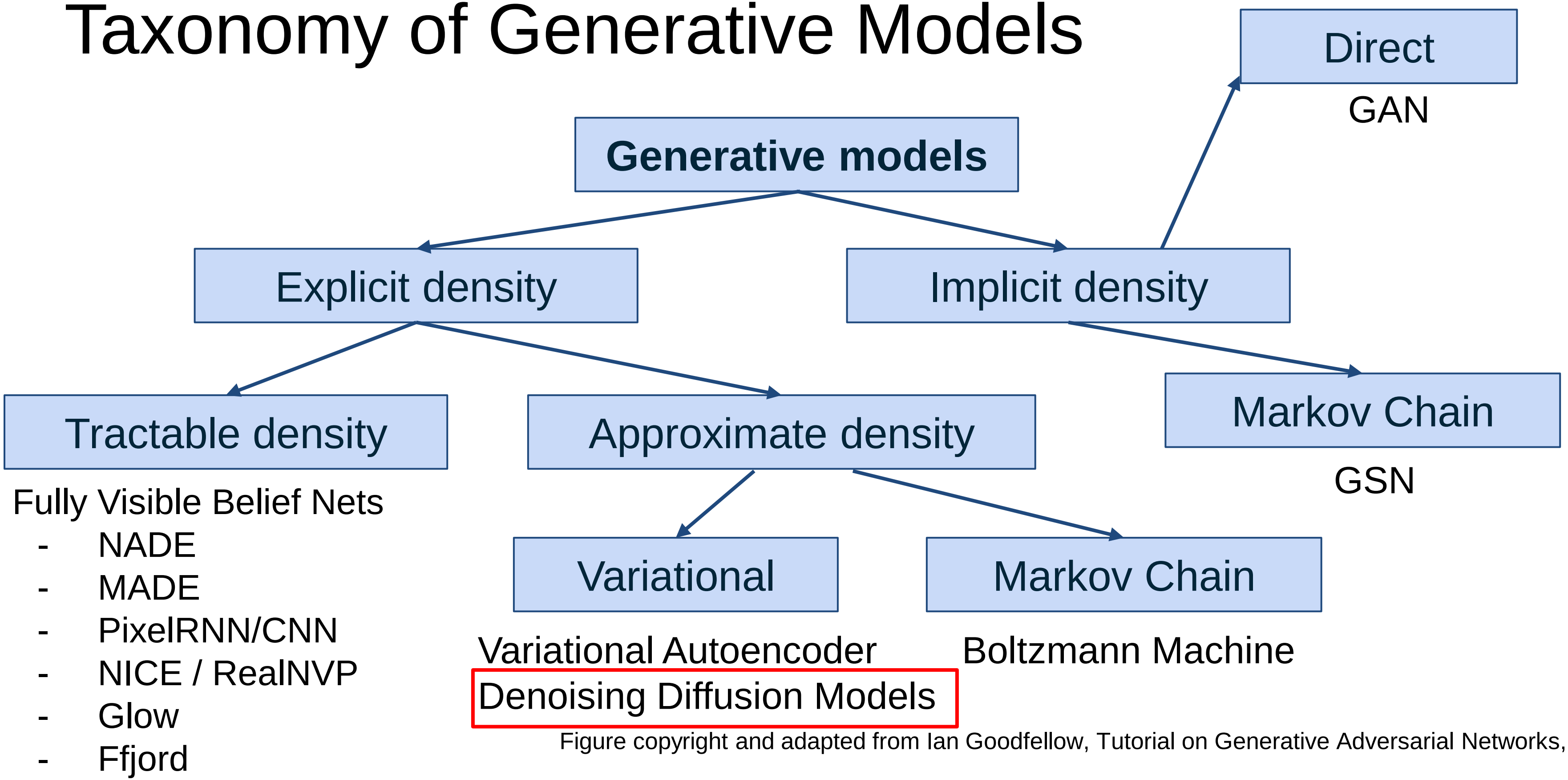


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

# Denoising Diffusion Probabilistic Models (DDPMs)

And Conditional Diffusion Models

TEXT DESCRIPTION

An astronaut Teddy bears A bowl of soup

riding a horse lounging in a tropical resort in space playing basketball with cats in space

in a photorealistic style in the style of Andy Warhol as a pencil drawing

→

DALL·E 2

https://openai.com/dall-e-2/

# Landscape Highlights of Diffusion Models (Nov 2022)

basic principles

- *Diffusion probabilistic models* (Sohl-Dickstein et al., 2015)
- *Noise-conditioned score network* (**NCSN**; Yang & Ermon, 2019)
- *Denoising diffusion probabilistic models* (**DDPM**; Ho et al. 2020)

conditional & high-res image generation

- *Classifier-guided conditional generation* (Dhariwal and Nichole, 2021)
- *Classifier-free Diffusion Guidance* (Ho and Salimans, 2022)
- *Latent-space Diffusion* (**StableDiffusion**; Rombach and Blattmann et al., 2022)

new applications

- *Planning with Diffusion for Flexible Behavior Synthesis* (**Diffuser**; Janner et al., 2022)
- *DreamFusion: Text-to-3D using 2D Diffusion* (Poole and Jain et al., 2022)
- *Make-A-Video: Text-to-Video Generation without Text-Video Data* (Singer et al., 2022)

# How to make a new generative model

- **Setting:** Given unlabeled dataset of data, I want to learn to sample from P(x)
- Define the generative process
- Parameterize it
- Maximum likelihood (often -> KL-divergence)
- Approximations
- Optimize parameters!
- Add conditioning, e.g. text

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# The Denoising Diffusion Process

image from
dataset

$x_0$

# The Denoising Diffusion Process

image from
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The "forward diffusion" process:
add Gaussian noise each step

$x_0$ → $x_1$ →

...

# The Denoising Diffusion Process

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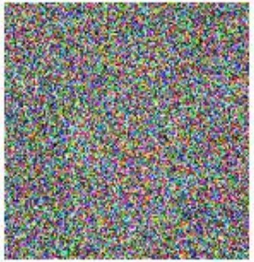
noise $\mathcal{N}(0, I)$

$x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_{T-1} \longrightarrow x_T$

...



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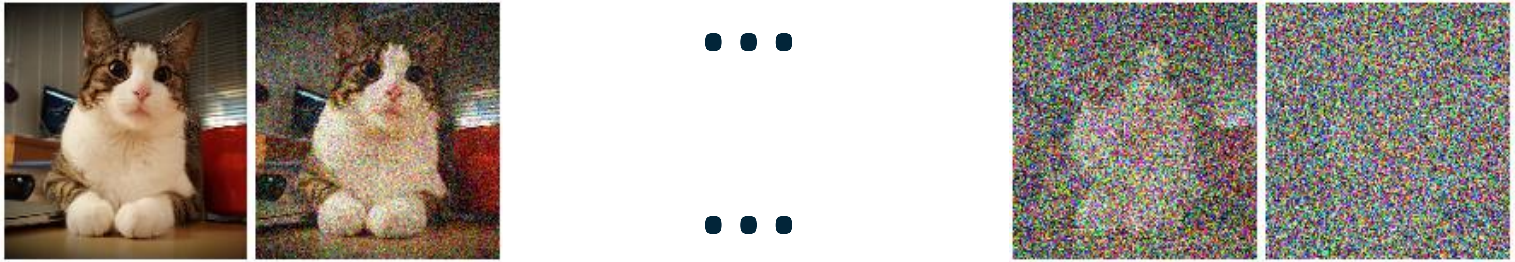
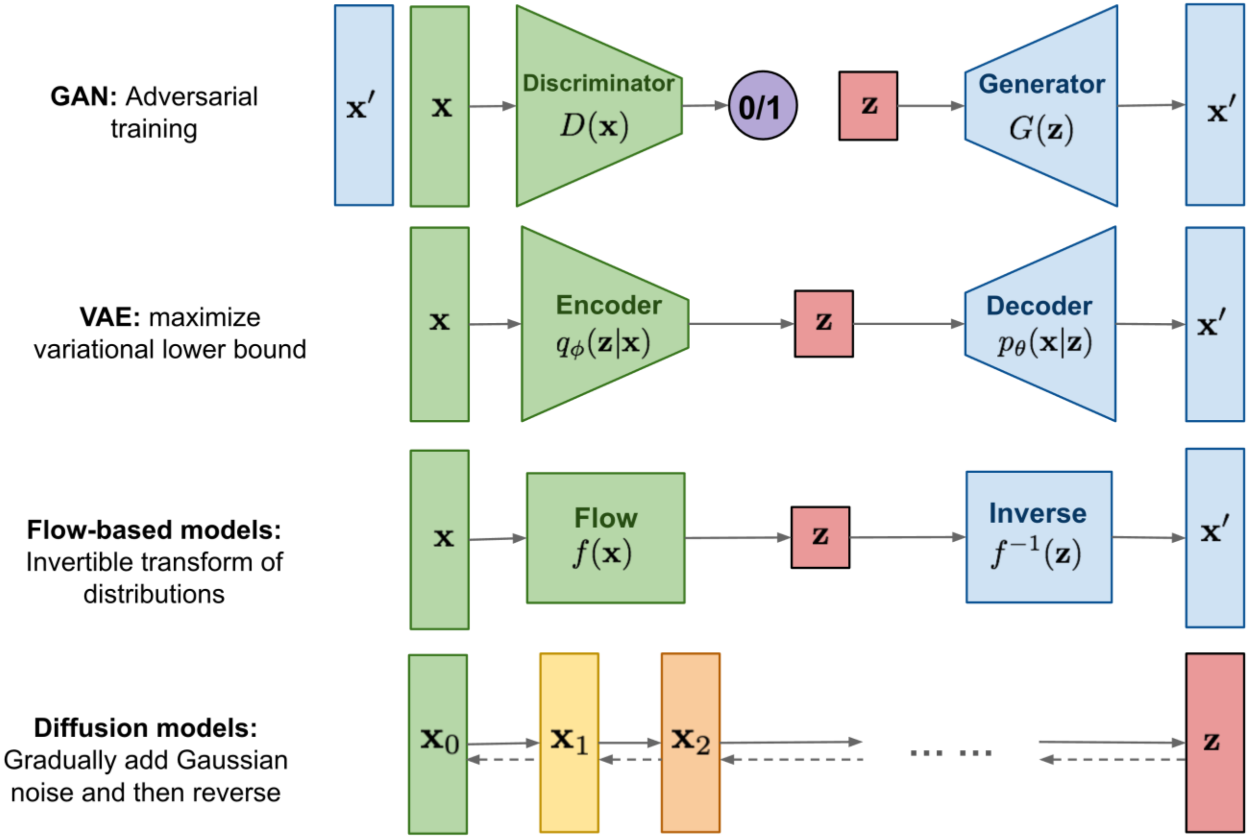


$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_{T-1} \leftarrow x_T$

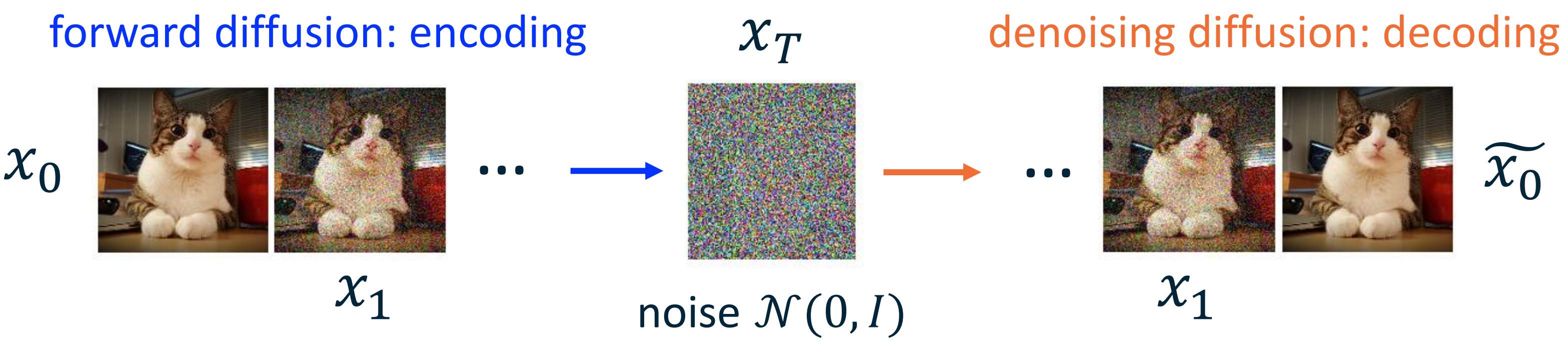
The "denoising diffusion" process: generate an image from noise by *denoising* the gaussian noises

Ties/inspiration form Annealed Imporantce Sampling in physics

# Comparison


**GAN:** Adversarial training
x′
x
Discriminator
$D(\mathbf{x})$
0/1
z
Generator
$G(\mathbf{z})$
x′
**VAE:** maximize variational lower bound
x
Encoder
$q_\phi(\mathbf{z}|\mathbf{x})$
z
Decoder
$p_\theta(\mathbf{x}|\mathbf{z})$
x′
**Flow-based models:** Invertible transform of distributions
x
Flow
$f(\mathbf{x})$
z
Inverse
$f^{-1}(\mathbf{z})$
x′
**Diffusion models:** Gradually add Gaussian noise and then reverse
$\mathbf{x}_0$
$\mathbf{x}_1$
$\mathbf{x}_2$
z

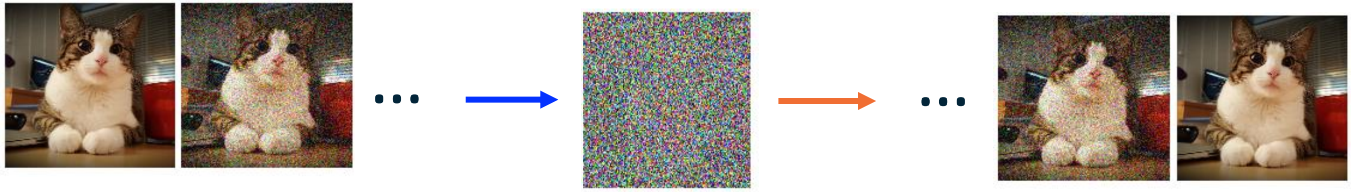
# Forward/Reverse Processes



# Forward/Reverse Processes

forward diffusion: encoding $x_T$ denoising diffusion: decoding

$x_0$



$\widetilde{x_0}$

$x_1$ noise $\mathcal{N}(0, I)$ $x_1$

Known / predefined:

$q(x_{1:T}|x_0)$

Unknown / learned:

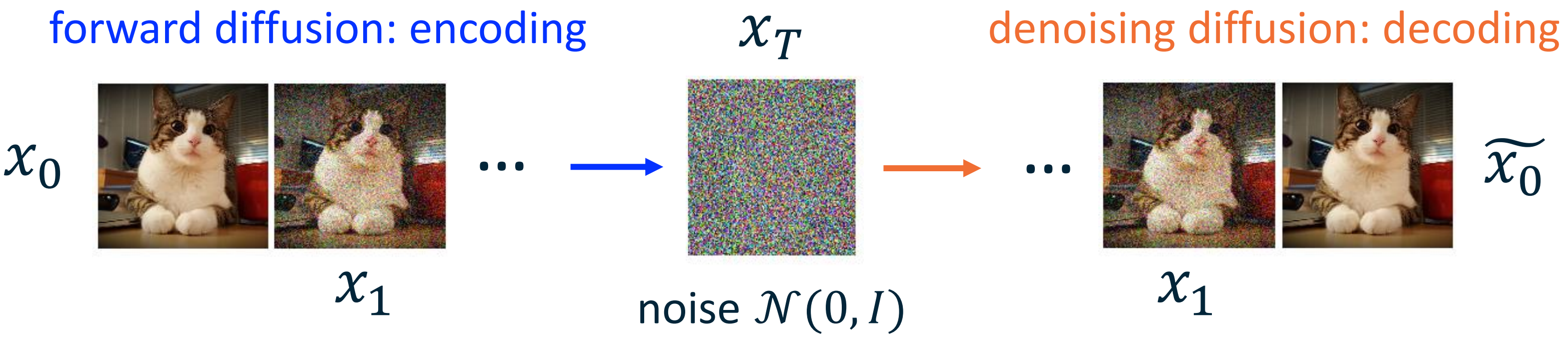
$$p_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

**Input:**

$x_t$


**Output: Noise mean to remove,** sample & use w/ $x_t$ to get $x_{t-1}$

# Forward/Reverse Processes

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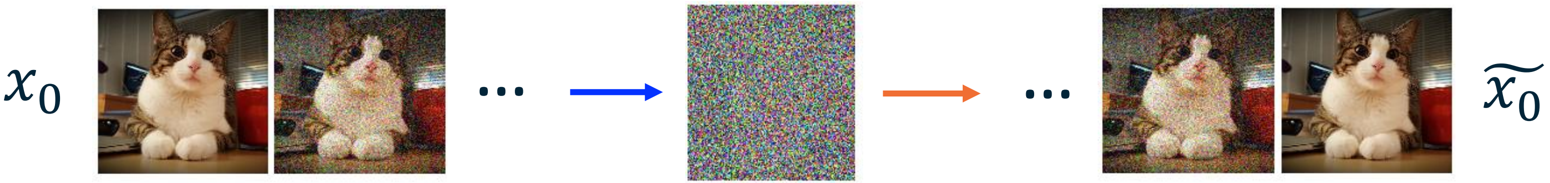
Use the denoising decoding process to generate new images.

# Forward/Reverse Processes

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The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \dots \longrightarrow x_T$

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Probability Chain Rule (Markov Chain)

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$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; (\sqrt{1-\beta_t})x_{t-1}, \beta_t I)$$ Conditional Gaussian

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Notation: A Gaussian distribution "for" $x_t$

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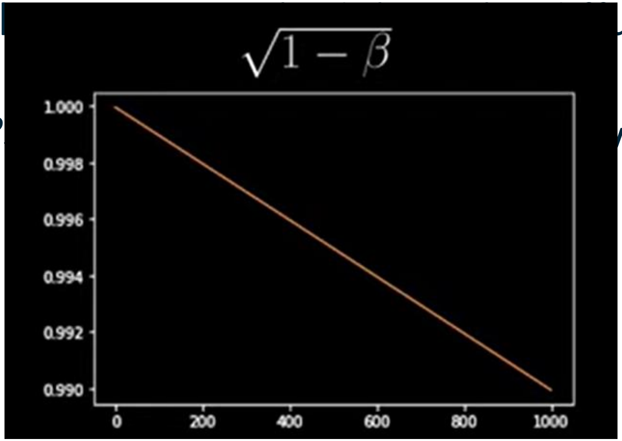
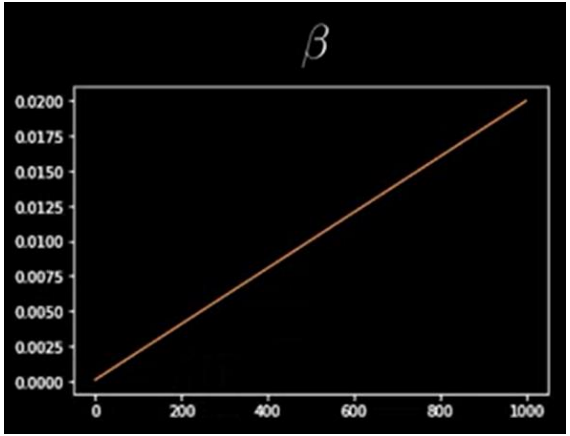
$\beta_t$ is t ... usion

$0 < \beta$ ... value ... $= 1000$




https://www.youtube.com/watch?v=HoKDTa5jHvg&t=517s

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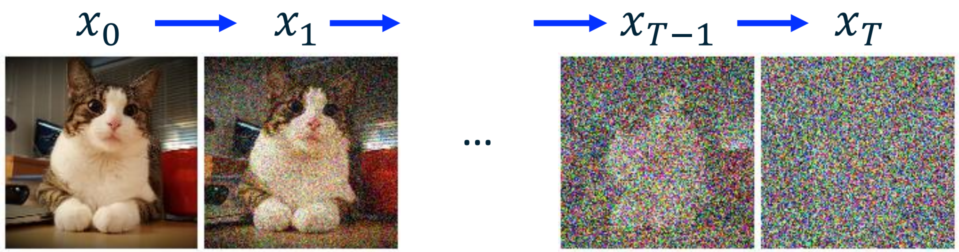
$\beta_t$ is the *variance schedule* at the diffusion step $t$

$0 < \beta_1 < \beta_2 < \cdots < \beta_T < 1$, typical value range $[0.0001, 0.02]$, with $T = 1000$



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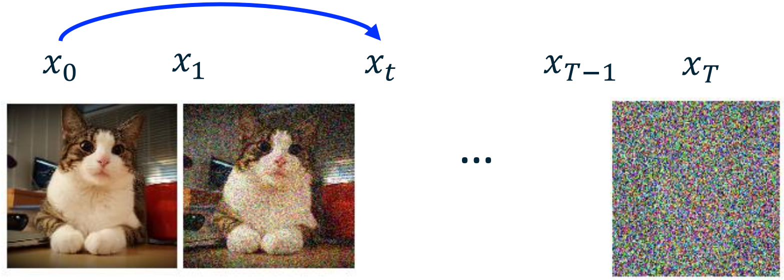
$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; (\sqrt{1-\beta_t})x_{t-1}, \beta_t I)$$ Conditional Gaussian

**Nice property**: samples from an *arbitrary forward step* are also Gaussian-distributed!

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)I)$$

, where $\alpha_t = (1-\beta_t)$, $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$



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$$\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$$

$$\begin{aligned}
\mathrm{q}(x_t|x_{t-1}) &= \mathcal{N}(x_t, \sqrt{1-\beta_t}x_{t-1}, \beta_t I) \\
&= \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon \\
&= \sqrt{\alpha_t}\, x_{t-1} + \sqrt{1-\alpha_t}\, \epsilon \\
&= \sqrt{\alpha_t \alpha_{t-1}}\, x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\, \epsilon \\
&= \sqrt{\alpha_t\alpha_{t-1}\alpha_{t-2}}\, x_{t-3} + \sqrt{1-\alpha_t\alpha_{t-1}\alpha_{t-2}}\, \epsilon \\
&= \sqrt{\alpha_t\alpha_{t-1}\dots\alpha_1\alpha_0}\, x_0 + \sqrt{1-\alpha_t\alpha_{t-1}\dots\alpha_1\alpha_0}\, \epsilon
\end{aligned}$$

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}\, x_0, (1-\bar{\alpha}_t)I) \longleftarrow \boxed{= \sqrt{\bar{\alpha}_t}\, x_0 + \sqrt{1-\bar{\alpha}_t}\, \epsilon}$$

# The Diffusion (Encoding

The **known** forward process $x_0$

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

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$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)I)$$

**Gaussian reparameterization trick**:

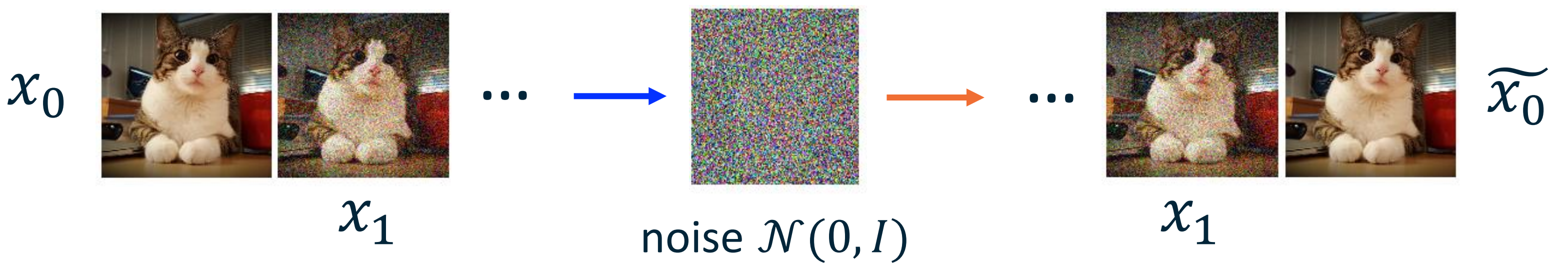
$$z = \mu + \epsilon * \sigma, \epsilon \sim N(0,1)$$

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, \qquad \epsilon \sim \mathcal{N}(0, I)$$

**Intuition: We know all distributions in forward process, and can in fact directly compute for any t based on $X_0$**

(square root appears because reparameterization trick has just $\sigma$)

# The Diffusion and Denoising Process

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$$p_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

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The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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Want to learn time-dependent mean

Assume fixed / known variance (simplification)

**What is the shape of the mean?**

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How do we form a learning objective?

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What does it look like? $q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

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← Recall: Gaussian reparameterization trick

The "ground truth" noise that brought $x_{t-1}$ to $x_t$

$$q(x_{t-1}|x_t) = \boldsymbol{q(x_{t-1}|x_t, x_0)} \quad \textbf{(markov assumption)}$$

$$= \frac{q(x_t|x_{t-1}, x_0)q(x_{t-1}|x_0)}{q(x_{t|}x_0)} \quad \text{(Bayes rule)}$$

$$= \frac{\mathcal{N}(x_t; \sqrt{a_t}x_{t-1}, \beta_t I)\mathcal{N}\left(x_{t-1}; \sqrt{\bar{\alpha}_{t-1}}x_{t-1}, (1-\bar{\alpha}_{t-1})I\right)}{\mathcal{N}\left(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_{t-1})I\right)}$$

$$\propto \mathcal{N}\left(x_{t-1}; \frac{\sqrt{a_t}(1-\bar{\alpha}_{t-1})x_t + \sqrt{\bar{\alpha}_{t-1}}(1-a_t)x_0}{1-\sqrt{\bar{\alpha}_t}}, \Sigma_q(t)\right) \quad \text{(Property of Gaussian)}$$

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$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right)$$

Assuming identical variance $\Sigma_q(t)$, we have:

$$\text{argmin}_\theta D_{KL}(q(x_{t-1}|x_t, x_0)\big|\big|p_\theta(x_{t-1}|x_t)) = \text{argmin}_\theta w||\mu_q(t) - \mu_\theta(x_t, t)||^2$$

Should be variance-dependent, but constant works better in practice

# The Denoising (Decoding) Process

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**Simplified learning objective:** $\text{argmin}_\theta ||\epsilon - \epsilon_\theta(x_t, t)||^2$

Predict the one-step noise that was added (and remove it)!

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$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_q(t))$$ Conditional Gaussian

Assume fixed / known variance

How did we arrive at the learning objective?
See slides at the end! Variational models …

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The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_q(t))$$

**Simplified learning objective:** $\mathbf{argmin}_\theta ||\epsilon - \epsilon_\theta(\boldsymbol{x}_t, \boldsymbol{t})||^2$

Predict the one-step noise that was added (and remove it)!

# The Denoising (Decoding) Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

Probability Chain Rule (Markov Chain)

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_q(t))$$

Conditional Gaussian

We know how to learn ($\mu_\theta(x_t, t)$)

Assume fixed / known variance ($\Sigma_q(t)$)

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

# The Denoising (Decoding) Process

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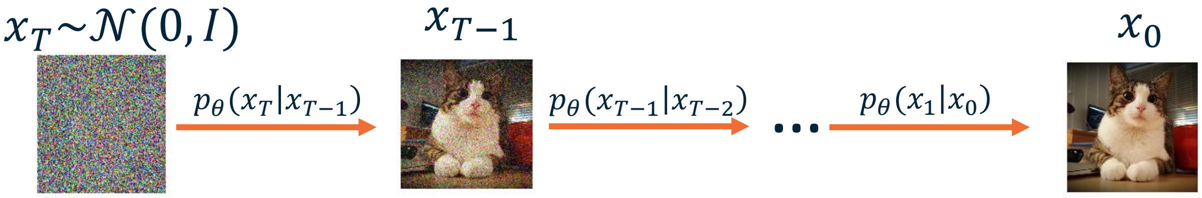


Generate new images!

# The Denoising Diffusion Algorithm

**Algorithm 1** Training

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

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

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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** $\mathbf{x}_0$

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

# The Denoising Diffusion Algorithm

**Algorithm 1** Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
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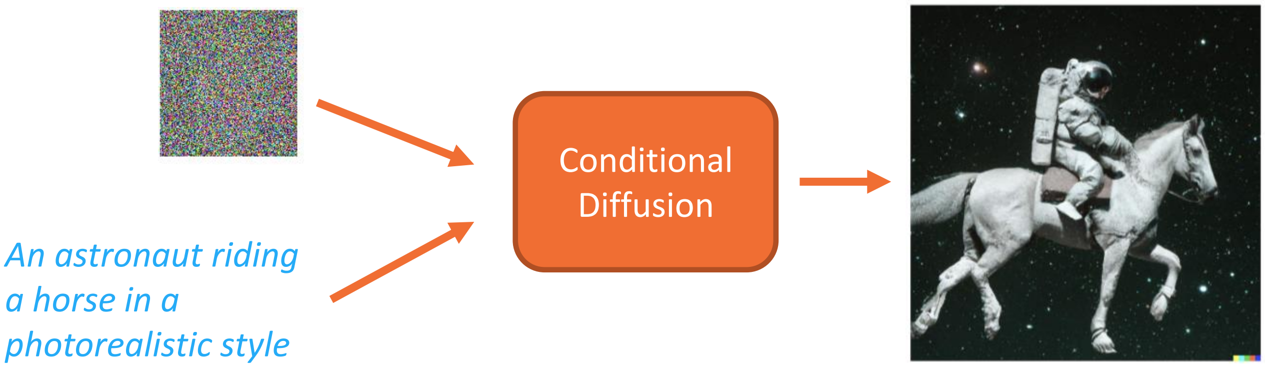
5: **end for**
6: **return** $\mathbf{x}_0$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma(t))$$

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, \qquad \epsilon \sim \mathcal{N}(0, I)$$

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

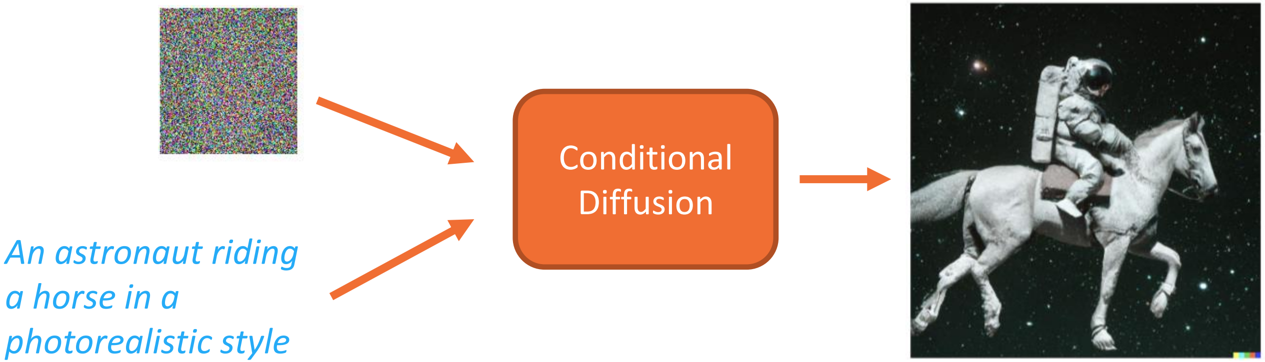
# Conditional Diffusion Models




Simple idea: just condition the model on some text labels $y$!

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

# Conditional Diffusion Models

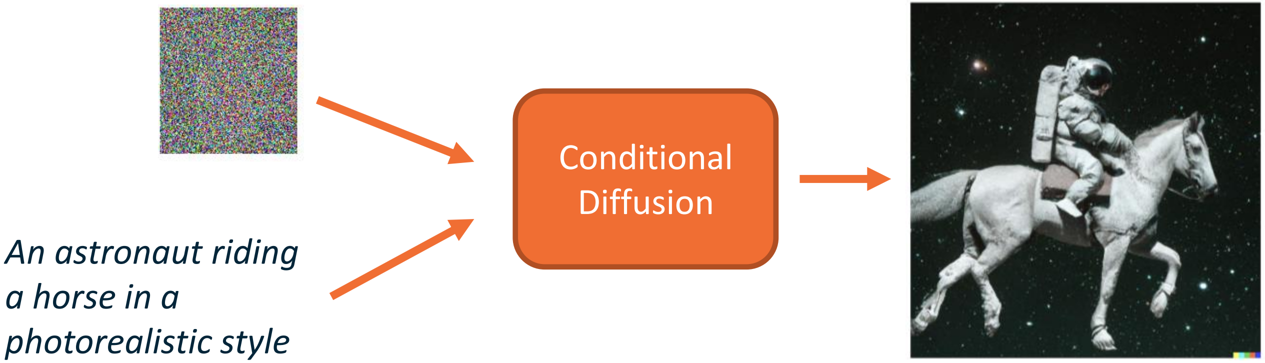



Simple idea: just condition the model on some text labels $y$!

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

Problem: Very blurry generation

# Classifier-guided Diffusion




Better idea: use the *gradients* from a image captioning model $f_\varphi(y|x_t)$ to guide the diffusion process!

$$\bar{\epsilon}_\theta(x_t, t) = \epsilon_\theta(x_t, t) - \sqrt{1 - \bar{\alpha}_t}\nabla_{x_t}\log f_\varphi(y|x_t)$$

Dhariwal & Nichol, 2021

# Classifier guidance

Using the gradient of a trained classifier as guidance

**Algorithm 1** Classifier guided diffusion sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $p_\phi(y|x_t)$, and gradient scale $s$.

Input: class label $y$, gradient scale $s$ — Score model — Classifier gradient
$x_T \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
**for all** $t$ from $T$ to 1 **do**
  $\mu, \Sigma \leftarrow \mu_\theta(x_t), \Sigma_\theta(x_t)$
  $x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + s\Sigma \nabla_{x_t} \log p_\phi(y|x_t), \Sigma)$
**end for**
**return** $x_0$

- Train unconditional Diffusion model

- Take your favorite classifier, depending on the conditioning type

- During inference / sampling mix the gradients of the classifier with the predicted score function of the unconditional diffusion model.

**Slide by Soumyadip (Roni) Sengupta**

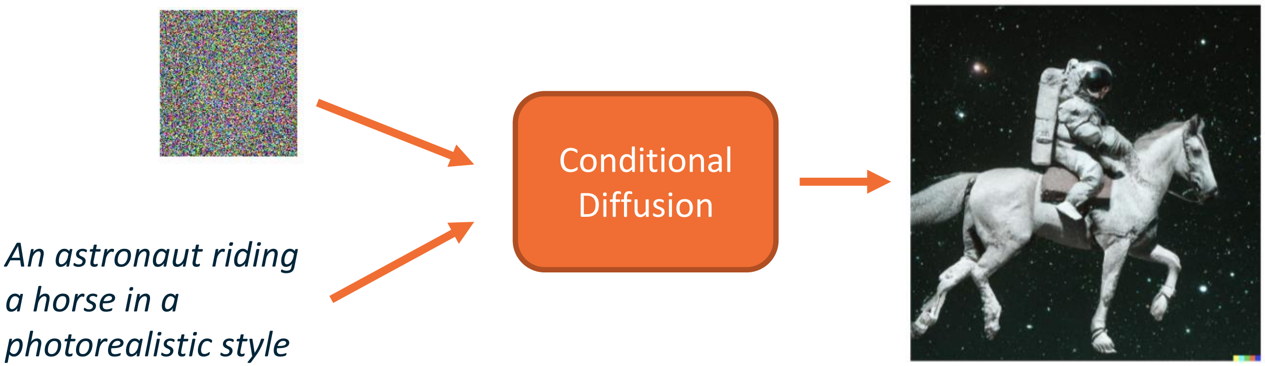
# Classifier guidance

Using the gradient of a trained classifier as guidance

$$\nabla_x \log p_\gamma(x \mid y) = \nabla_x \log p(x) + \gamma \nabla_x \log p(y \mid x).$$

Samples from an unconditional diffusion model with classifier guidance, for guidance scales 1.0 (left) and 10.0 (right), taken from Dhariwal & Nichol (2021).

# Classifier-free Guided Diffusion




**Classifier-free Guided Diffusion**: estimate the gradient of the classifier model with conditional diffusion models!

$$\nabla_{x_t} \log f_\varphi(y|x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}}(\epsilon_\theta(x_t, t, y) - \epsilon_\theta(x_t, t))$$

Ho and Salimans, 2022

# Classifier-free guidance

Trade-off for sample quality and sample diversity

Non-guidance

Guidance scale = 1

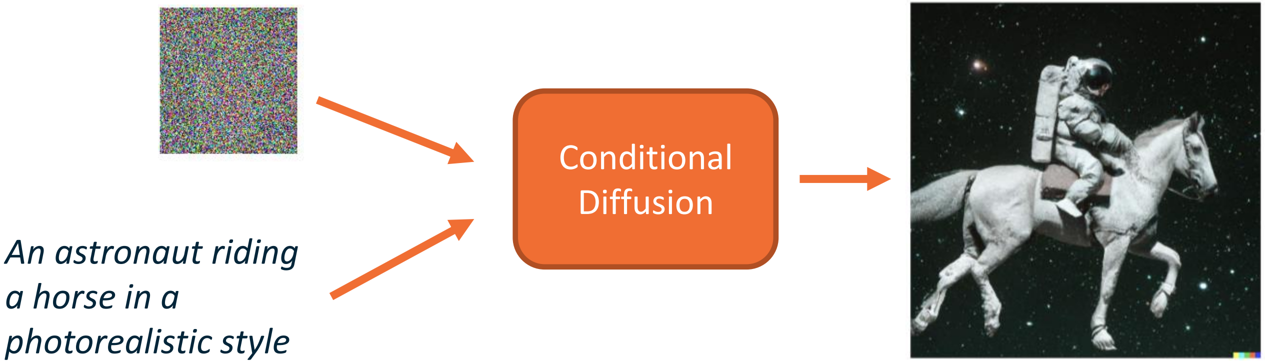
Guidance scale = 3

Large guidance weight ($\omega$) usually leads to better individual sample quality but less sample diversity.

Ho & Salimans, "Classifier-Free Diffusion Guidance", 2021.

**Slide by Soumyadip (Roni) Sengupta**

# Classifier-free Guided Diffusion

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$$\nabla_{x_t} \log f_\varphi(y|x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}}\left(\epsilon_\theta(x_t, t, y) - \epsilon_\theta(x_t, t)\right)$$

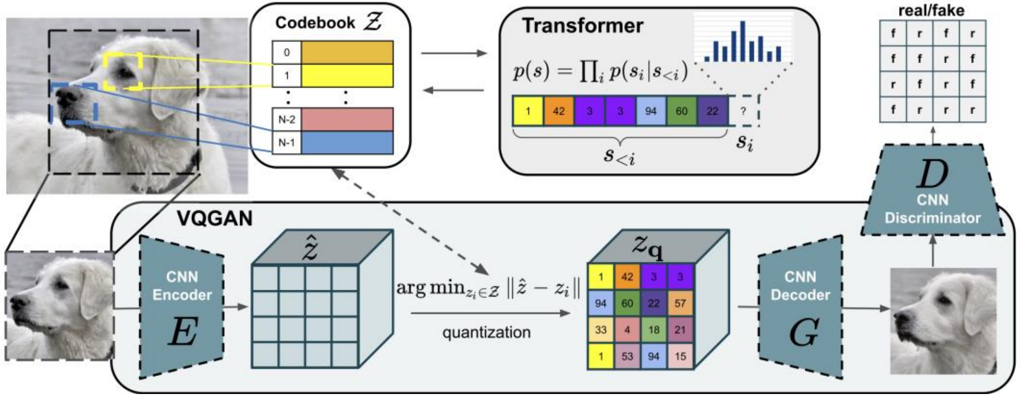
$$\bar{\epsilon}_\theta(x_t, t, y) = (w+1)\epsilon_\theta(x_t, t, y) - w\epsilon_\theta(x_t, t)$$

Ho and Salimans, 2022

# Latent-space Diffusion

Problem: Hard to learn diffusion process on high-resolution images

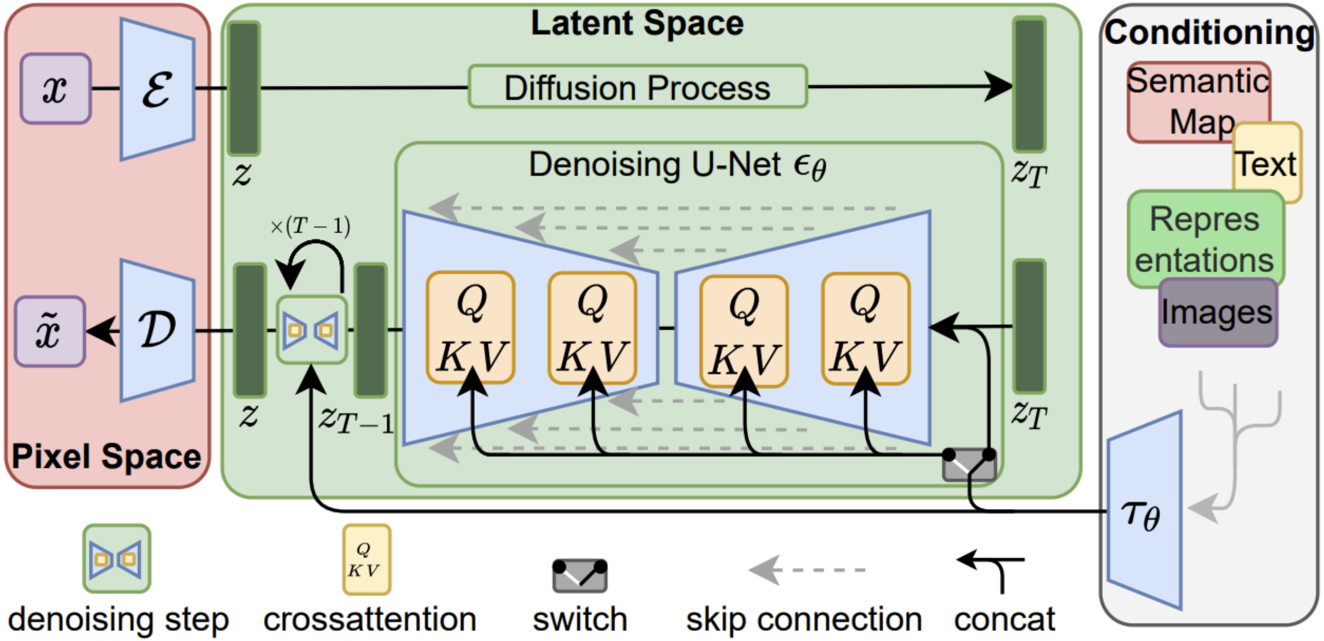
Solution: learn a low-dimensional latent space using a transformer-based autoencoder and *do diffusion on the latent space*!




The latent space autoencoder

Esser and Rombach *et al.*, 2021

# "StableDiffusion"




Rombach and Blattmann *et al.*, 2022

# “StableDiffusion”


Layout-Conditional Generation

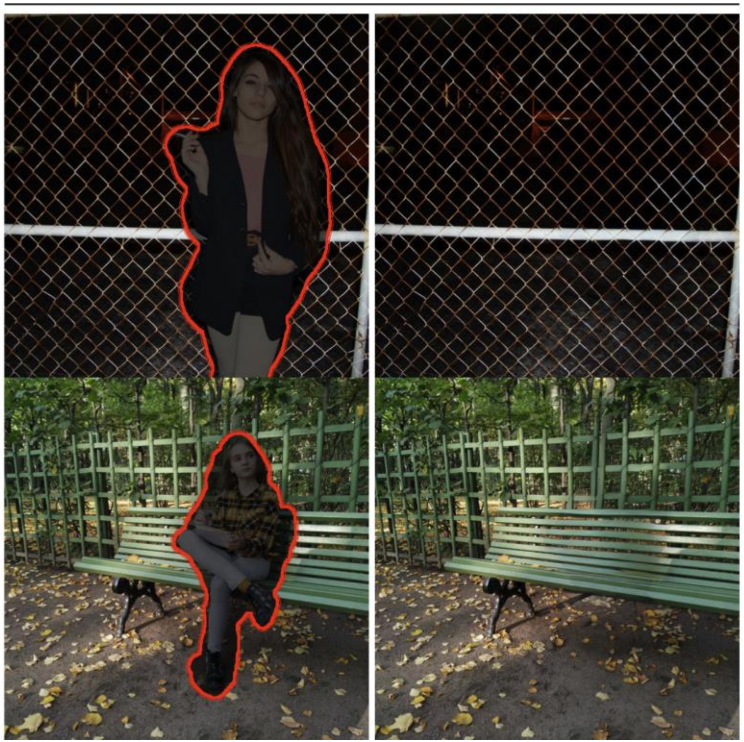
Rombach and Blattmann *et al.*, 2022

# “StableDiffusion”

Segmentation-Conditional Generation

Rombach and Blattmann *et al.*, 2022

# “StableDiffusion”



Inpainting

Rombach and Blattmann *et al.*, 2022

https://openai.com/dall-e-2/

# Additional resources / tutorials

- Overview of the research landscape: What are Diffusion Models?
- More math! Understanding Diffusion Models: A Unified Perspective
- Tutorial with hands-on example: The Annotated Diffusion Model
- Nice introduction videos:
  - What are Diffusion Models?
  - Diffusion Models | Math Explained
  - Three hours of the math! https://www.youtube.com/watch?v=rLepfNziDPM
- CVPR Tutorial: Denoising Diffusion-based Generative Modeling: Foundations and Applications
- Score functions:
  - In general
  - For Diffusion models

# Summary

- Denoising Diffusion model is a type of generative model that learns the process of “denoising” a known noise source (Gaussian).
- We can construct a learning problem by deriving the evidence lower bound (ELBO) of the denoising process.
- The learning objective is to minimize the KL divergence between the “ground truth” and the learned denoising distribution.
- A simplified learning objective is to estimate the noise of the forward diffusion process.
- The diffusion process can be guided to generate targeted samples.
- Can be applied to many different domains. Same underlying principle.
- Very hot topic!

# (Quick) Derivation!

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization → Remove (variance-dependent) constant → Predict the noise!!!

$p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!

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

**Variational Inference**

$p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!

$$\log p(x) = \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right] + D_{KL}(q(z|x)||p(z|x))$$

$$\geq \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right]$$ Evidence Lower Bound (ELBO)

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$$\log p(x_0) \geq \mathrm{E}_q\left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

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… (derivation omitted, see Sohl-Dickstein *et al.,* 2015 Appendix B)

$$= \mathrm{E}_q\left[\log\frac{p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)}{\prod_{t=1}^{T} q(x_t|x_{t-1})}\right]$$

← reverse denoising

← forward diffusion

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

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… (derivation omitted, see Sohl-Dickstein *et al.,* 2015 Appendix B)

$$= -\mathrm{E}_q[D_{KL}(q(x_T|x_0)||p(x_T))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) + \log p_\theta(x_0|x_1)$$

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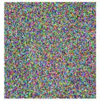
fixed



Easy to optimize / sometimes omitted

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

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Maximize the agreement between the predicted reverse diffusion distribution $p_\theta$ and the "ground truth" reverse diffusion distribution $q$

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

Variational Inference → Simplify to KL → Reverse Process => Normal

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$q(x_{t-1}|x_t) = \boldsymbol{q(x_{t-1}|x_t,x_0)}$ **(markov assumption)**

$$= \frac{q(x_t|x_{t-1},x_0)q(x_{t-1}|x_0)}{q(x_t|x_0)}$$ (Bayes rule)

$$= \frac{\mathcal{N}(x_t;\sqrt{\alpha_t}x_{t-1},\beta_t I)\mathcal{N}(x_{t-1};\sqrt{\bar{\alpha}_{t-1}}x_{t-1},(1-\bar{\alpha}_{t-1})I)}{\mathcal{N}(x_t;\sqrt{\bar{\alpha}_t}x_0,(1-\bar{\alpha}_{t-1})I)}$$

$$\propto \mathcal{N}\left(x_{t-1};\ \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t+\sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)x_0}{1-\sqrt{\bar{\alpha}_t}}, \Sigma_q(t)\right)$$ (Property of Gaussian)

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

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$x = x_0, \; z = x_{1:T}$

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$$q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

Proof using bayes rule and gaussian reparameterization trick

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

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$$= -\mathrm{E}_q[D_{KL}(q(x_T|x_0)||p(x_T))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) + \log p_\theta(x_0|x_1)$$

$$q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \quad \epsilon \sim \mathcal{N}(0, I)$$

Proof using bayes rule and gaussian reparameterization trick

The "ground truth" noise that brought $x_{t-1}$ to $x_t$

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

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization → Remove (variance-dependent) constant

$p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!

$$\log p(x) = \mathrm{E}_q\left[\log\frac{p(x|z)p(z)}{q(z|x)}\right] + D_{KL}(q(z|x)||p(z|x))$$

$$\geq \mathrm{E}_q\left[\log\frac{p(x|z)p(z)}{q(z|x)}\right]$$ Evidence Lower Bound (ELBO)

$$\log p(x_0) \geq \mathrm{E}_q\left[\log\frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

… (derivation omitted, see Sohl-Dickstein *et al.*, 2015 Appendix B)

$$= -\mathrm{E}_q[D_{KL}(q(x_T|x_0)||p(x_T))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) + \log p_\theta(x_0|x_1)$$

Minimize the difference of distribution means (assuming identical variance)

$$\mathrm{argmin}_\theta w||\mu_q(t) - \mu_\theta(x_t, t)||^2$$

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization → Remove (variance-dependent) constant → Predict the noise!!!

# Learning the Denoising Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

$$p_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma(t))$$

Conditional Gaussian

Learning objective: $\operatorname{argmin}_\theta ||\mu_q(t) - \mu_\theta(x_t, t)||^2$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

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$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

Do we actually need to learn the entire $\mu_\theta(x_t, t)$?

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization → Remove (variance-dependent) constant → Predict the noise!!!

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known during inference

Unknown during inference

Recall: this is the “ground truth” noise that brought $x_{t-1}$ to $x_t$

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Conditional Gaussian

Learning objective: $\text{argmin}_\theta ||\mu_q(t) - \mu_\theta(x_t, t)||^2$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

known during inference

Unknown during inference

Recall: this is the "ground truth" noise that brought $x_{t-1}$ to $x_t$

Idea: just learn $\epsilon$ with $\epsilon_\theta(x_t, t)$!

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization → Remove (variance-dependent) constant → Predict the noise!!!

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Conditional Gaussian

Simplified learning objective: $\text{argmin}_\theta ||\epsilon - \epsilon_\theta(x_t, t)||^2$

# Learning the Denoising Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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Simplified learning objective: $\text{argmin}_\theta ||\epsilon - \epsilon_\theta(x_t, t)||^2$

Recall: the simplified $t$-step forward sample:

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon$$

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization → Remove (variance-dependent) constant → Predict the noise!!!

# Learning the Denoising Process

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$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma(t))$$

Conditional Gaussian

Simplified learning objective: $\text{argmin}_\theta ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2$

Recall: the simplified $t$-step forward sample:

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$$

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Simplified learning objective: $\text{argmin}_\theta ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2$

# Math for Classifier Guidance

# Conditional diffusion models

Include condition as input to reverse process

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

Variational upper bound: $L_\theta(\mathbf{x}_0|\mathbf{c}) = \mathbb{E}_q\left[L_T(\mathbf{x}_0) + \sum_{t>1} D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{c})) - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1, \mathbf{c})\right].$

Incorporate conditions into U-Net

- Scalar conditioning: encode scalar as a vector embedding, simple spatial addition or adaptive group normalization layers.
- Image conditioning: channel-wise concatenation of the conditional image.
- Text conditioning: single vector embedding - spatial addition or adaptive group norm / a seq of vector embeddings - cross-attention.



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# Classifier guidance

Using the gradient of a trained classifier as guidance

Applying Bayes rule to obtain conditional score function $\nabla_{x_t} log\ q_t(x_t/y)$

$$p(x \mid y) = \frac{p(y \mid x) \cdot p(x)}{p(y)}$$

$$\implies \log p(x \mid y) = \log p(y \mid x) + \log p(x) - \log p(y)$$

$$\implies \nabla_x \log p(x \mid y) = \nabla_x \log p(y \mid x) + \nabla_x \log p(x),$$

$$\nabla_x \log p_\gamma(x \mid y) = \nabla_x \log p(x) + \gamma \nabla_x \log p(y \mid x).$$ ← Classifier

Guidance scale: value >1 amplifies the influence of classifier signal.

$$p_\gamma(x \mid y) \propto p(x) \cdot p(y \mid x)^\gamma.$$

Slide Credits of guidance: https://benanne.github.io/2022/05/26/guidance.html

# Classifier guidance

## Problems of classifier guidance

$$\nabla_x \log p_\gamma(x \mid y) = \nabla_x \log p(x) + \gamma \nabla_x \log p(y \mid x).$$ ← Classifier

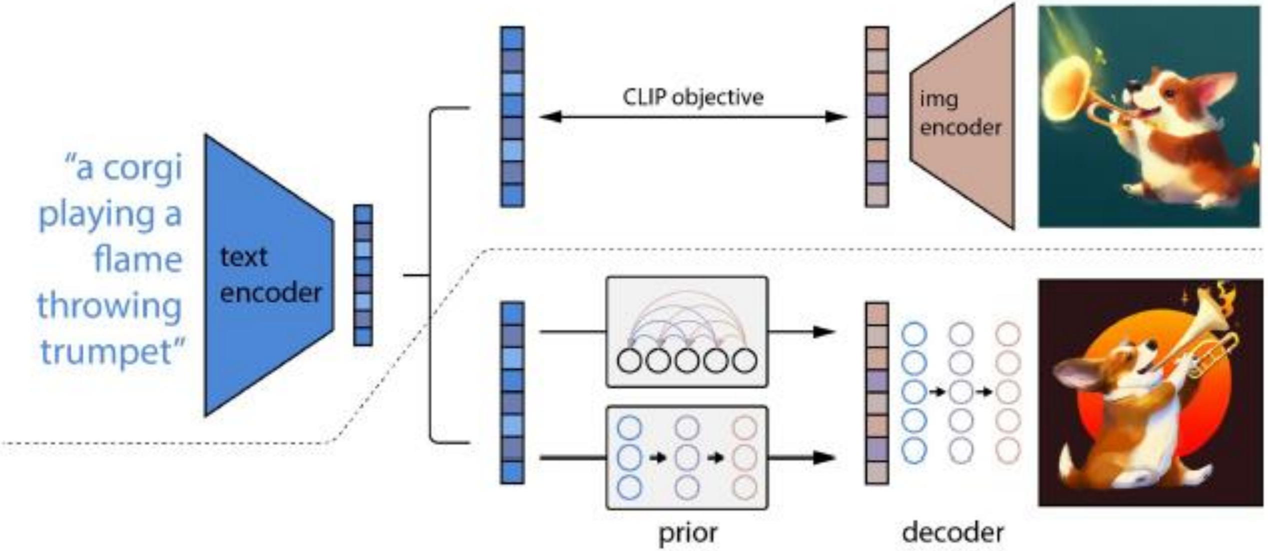
Guidance scale: value >1 amplifies the influence of classifier signal.

- At each step of denoising the input to the classifier is a noisy image $x_t$ . Classifier is never trained on noisy image. So one needs to re-train classifier on noisy images! Can't use existing pre-trained classifiers.
- Most of the information in the input x is not relevant to predicting y, and as a result, taking the gradient of the classifier w.r.t. its input can yield arbitrary (and even adversarial) directions in input space.

Solution 1 (DALL-E 2): Use CLIP Model

# DALL·E 2

## Model components




Why conditional on CLIP image embeddings?

CLIP image embeddings capture high-level semantic meaning.

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# Classifier-free guidance

Get guidance by Bayes' rule on conditional diffusion models

$$p(y \mid x) = \frac{p(x \mid y) \cdot p(y)}{p(x)}$$

$$\implies \log p(y \mid x) = \log p(x \mid y) + \log p(y) - \log p(x)$$

$$\implies \nabla_x \log p(y \mid x) = \nabla_x \log p(x \mid y) - \nabla_x \log p(x).$$

We proved this in classifier guidance.

$$\nabla_x \log p_\gamma(x \mid y) = \nabla_x \log p(x) + \gamma \nabla_x \log p(y \mid x).$$

$$\nabla_x \log p_\gamma(x \mid y) = \nabla_x \log p(x) + \gamma \left( \nabla_x \log p(x \mid y) - \nabla_x \log p(x) \right),$$

$$\nabla_x \log p_\gamma(x \mid y) = (1 - \gamma) \nabla_x \log p(x) + \gamma \nabla_x \log p(x \mid y).$$

$(1 - \gamma) \nabla_x \log p(x)$: Score function for unconditional diffusion model

$\gamma \nabla_x \log p(x \mid y)$: Score function for conditional diffusion model

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# Classifier-free guidance

Get guidance by Bayes' rule on conditional diffusion models

$$\hat{\epsilon} = (1+\omega)\epsilon_\theta(x_t, y) - \omega\epsilon_\theta(x_t)$$

$$\nabla_x \log p_\gamma(x \mid y) = (1-\gamma)\nabla_x \log p(x) + \gamma\nabla_x \log p(x \mid y).$$

Score function for unconditional diffusion model

Score function for conditional diffusio model

In practice:

- Train a conditional diffusion model p(x|y), with *conditioning dropout*: some percentage of the time, the conditioning information y is removed (10-20% tends to work well).
- The conditioning is often replaced with a special input value representing the absence of conditioning information.
- The resulting model is now able to function both as a conditional model p(x|y), and as an unconditional model p(x), depending on whether the conditioning signal is provided.
- During inference / sampling simply mix the score function of conditional and unconditional diffusion model based on guidance scale.