

# Diffusion Models and an application to DALL-E2

## Deep Learning and Neural Networks: Advanced Topics

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*Retis*  
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Introduction

Diffusion Models

DALL-E2

Conclusion

## Introduction

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# Generative Models

**1D example:**  
we illustrate the  
effet of G over  
the entire  
distribution

*Generative model  
to be learned*

*Simple 1D gaussian  
distribution we know  
how to sample from*

*Targeted complex 1D  
distribution we don't know  
how to sample from*

$$G(\text{---}) = \text{---}$$

**High dimension  
example:**  
we illustrate the  
effet of G over a  
single sample

$$G(\text{---}) = \text{---}$$



*Generative model  
to be learned*

*High dimension data  
point from simple  
noise distribution*

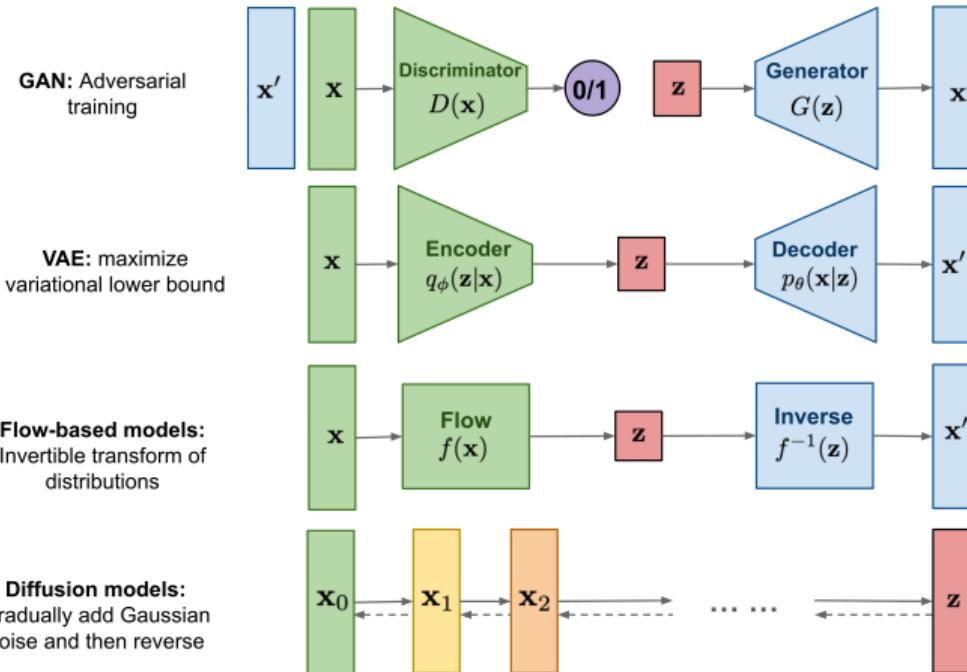
*High dimension data  
point from complex  
image distribution*

Schema of generative models<sup>1</sup>

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<sup>1</sup>Credits: <https://towardsdatascience.com/understanding-diffusion-probabilistic-models-dpms-1940329d6048>

# Generative Models



Overview of different generative models<sup>2</sup>

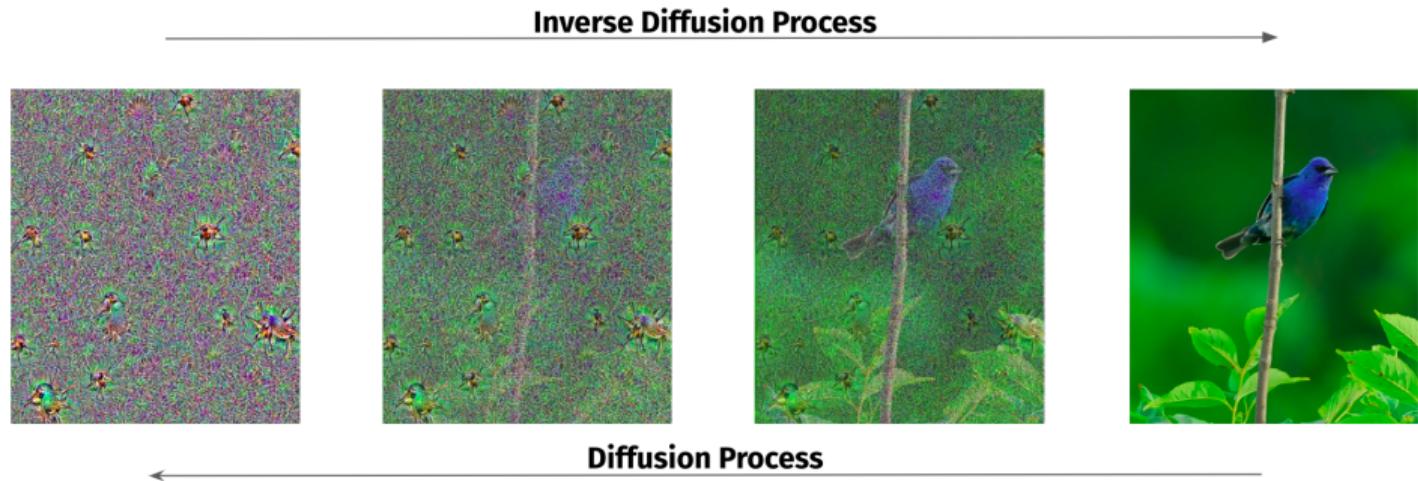
<sup>2</sup>Credits <https://lilianweng.github.io/posts/2021-07-11-diffusion-models/>

## Diffusion Models

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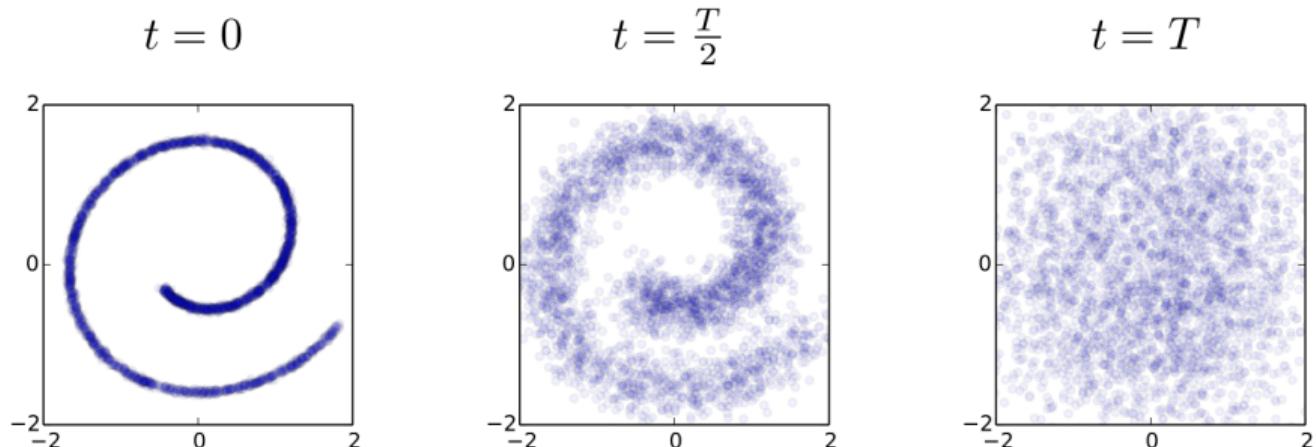
*Diffusion models are generative models that aim at denoising data*



## Timeline

- 2015) *Deep Unsupervised Learning with Non-equilibrium Thermodynamics*. Sohl-Dickstein et al. ICML.
- 2020) *Denoising Diffusion Probabilistic Models*. Ho et al. NeurIPS.
- 2021) *Score-Based Generative Modeling Through SDE*. Song et al. ICLR.

# Deep Unsupervised Learning using Non-Equilibrium Thermodynamics



Diffusion process as a **Markov Chain** with Continuous State Space and Discrete Time.<sup>3</sup>

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<sup>3</sup>Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

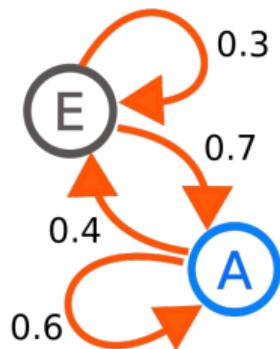
# Reminder: Markov Chains with Discrete Time

## Informal Definition

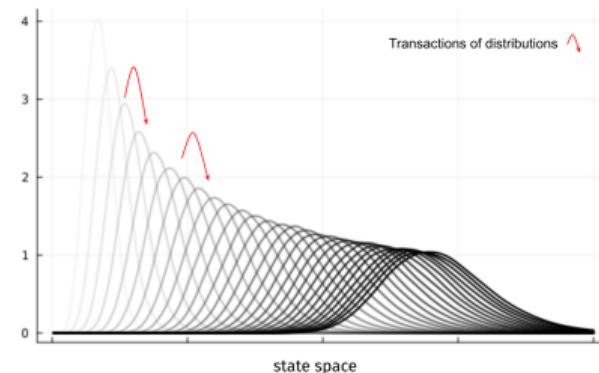
A sequence of random variables  $x^{(0)}, x^{(1)}, \dots, x^{(t)}, \dots$ , such that

- $x^{(t)} \in S$ , where  $S$  State Space
- The future  $x^{(t+1)}$  depends on the present  $x^{(t)}$  but not on the past  $x^{(t-1)}$

Discrete State Space  $S$



Continuous State Space  $S$



## Reminder: Discrete Time Markov Chain with Discrete State Space

### Definition

A sequence  $\left\{ \mathbf{x}^{(t)} \right\}_{t \in \mathbb{N}} \subseteq S$ , a matrix  $P = (p_{ij})$ .

- Discrete state space:  $S = \{s_0, \dots, s_n, \dots\}$
- Markov Property:  $\mathbf{x}^{(t+1)}$  not dep.  $\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(t-1)}$ .
- Transition Matrix:  $\mathbb{P}\left(\mathbf{x}^{(t+1)} = s_j | \mathbf{x}^{(t)} = s_i\right) = p_{ij}$

# Reminder: Discrete Time Markov Chain with Discrete State Space

## Definition

A sequence  $\{\mathbf{x}^{(t)}\}_{t \in \mathbb{N}} \subseteq S$ , a matrix  $P = (p_{ij})$ .

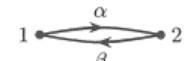
$P$  is a stochastic matrix!

$$\forall i, \quad \sum_{j \in \mathbb{N}} p_{ij} = 1$$

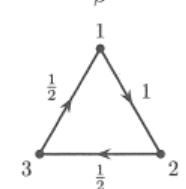
- Discrete state space:  $S = \{s_0, \dots, s_n, \dots\}$

- Markov Property:  $\mathbf{x}^{(t+1)}$  not dep.  $\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(t-1)}$ .

$$P = \begin{pmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{pmatrix}$$



$$P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \end{pmatrix}$$



- Transition Matrix:  $\mathbb{P}(\mathbf{x}^{(t+1)} = s_j | \mathbf{x}^{(t)} = s_i) = p_{ij}$

## Reminder: DTMC with Continuous State Space

Let assume  $\mathbf{x}, \mathbf{y} \in S$  where  $S$  continuous state space (e.g.  $S = \mathbb{R}^d$ ).

Joint Distribution  $p(\mathbf{x}, \mathbf{y})$

$$\mathbb{P}(\mathbf{x} \in A \mid \mathbf{y} \in B) = \int_A \int_B p(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \, d\mathbf{y}$$

Transactional Kernel  $p(\mathbf{x} \mid \mathbf{y})$

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x} \mid \mathbf{y}) p(\mathbf{y})$$

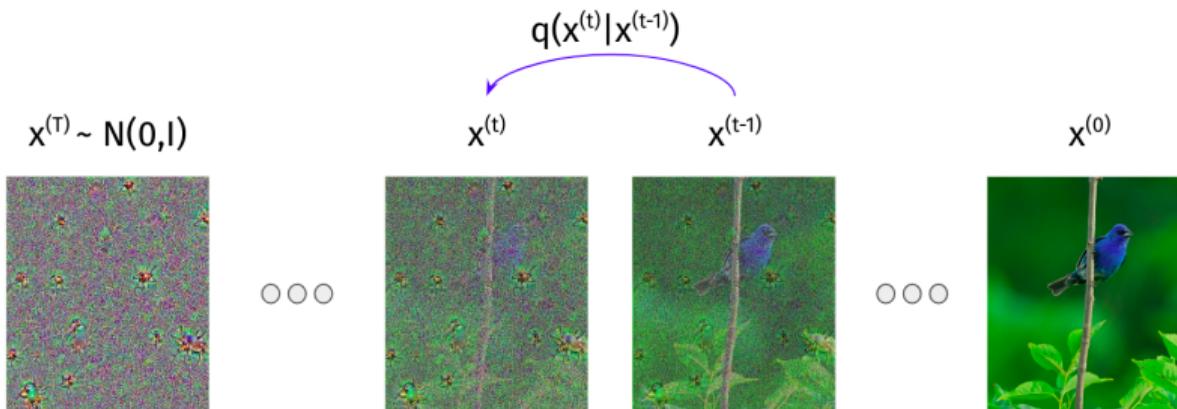
Marginal Distribution  $p(\mathbf{x})$

$$p(\mathbf{x}) = \int_S p(\mathbf{x}, \mathbf{y}) \, d\mathbf{y} = \int_S p(\mathbf{x} \mid \mathbf{y}) p(\mathbf{y}) \, d\mathbf{y}$$

# Forward Diffusion Process

“Adding noise to data...”

- Data Distribution:  $\mathbf{x}^{(0)} \sim q$
- Transaction Kernel:  $q\left(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)}\right) = \mathcal{N}\left(\mathbf{x}^{(t)}; \sqrt{1 - \beta_t} \mathbf{x}^{(t-1)}; \beta_t I\right)$
- Variance Scheduler:  $0 < \beta_1 < \dots < \beta_T < 1$

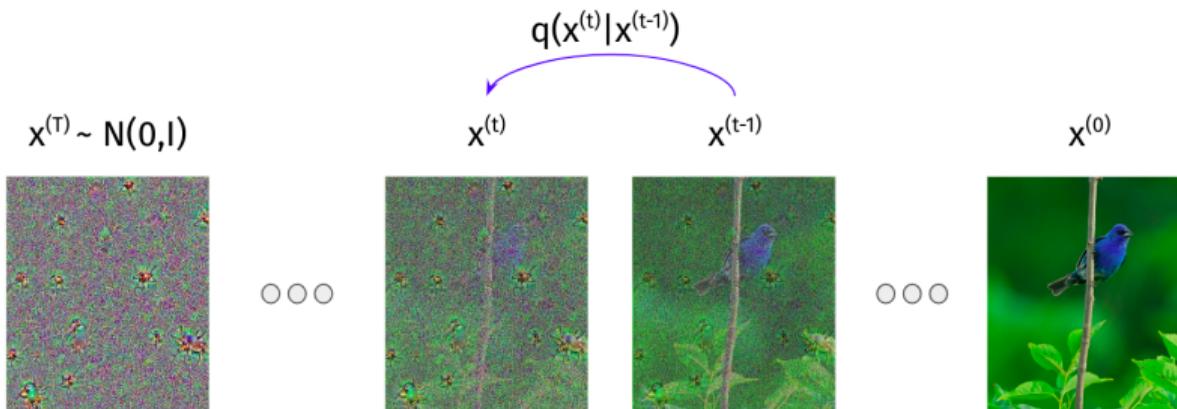


# Forward Diffusion Process

“Adding noise to data...”

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- Variance Scheduler:  $0 < \beta_1 < \dots < \beta_T < 1$

Not Analytic!!



## Forward Diffusion Process: Explicit Representation

$$\mathbf{x}^{(t)} = \sqrt{1 - \beta_t} \mathbf{x}^{(t-1)} + \sqrt{\beta_t} \boldsymbol{\varepsilon}_t, \quad \boldsymbol{\varepsilon}_t \sim \mathcal{N}(0, I)$$

Observation: Many small noisy steps  $\approx$  Large Noisy step

$$\mathbf{x}^{(t)} = \sqrt{1 - \alpha_t} \mathbf{x}^{(0)} + \sqrt{\alpha_t} \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(0, I)$$

where

$$\alpha_t = 1 - \prod_{i=0}^t (1 - \beta_i)$$

## Forward Diffusion Process: Distribution Representation

Markov property allows breaking up distributional Representation...

$$q(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T)}) = q\left(\mathbf{x}^{(T)} \mid \mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right) q\left(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right)$$

## Forward Diffusion Process: Distribution Representation

Markov property allows breaking up distributional Representation...

$$\begin{aligned} q(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T)}) &= q\left(\mathbf{x}^{(T)} \mid \mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right) q\left(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right) \\ &= q\left(\mathbf{x}^{(T)} \mid \mathbf{x}^{(T-1)}\right) q\left(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right) \\ &\vdots \end{aligned} \tag{1}$$

## Forward Diffusion Process: Distributional Representation

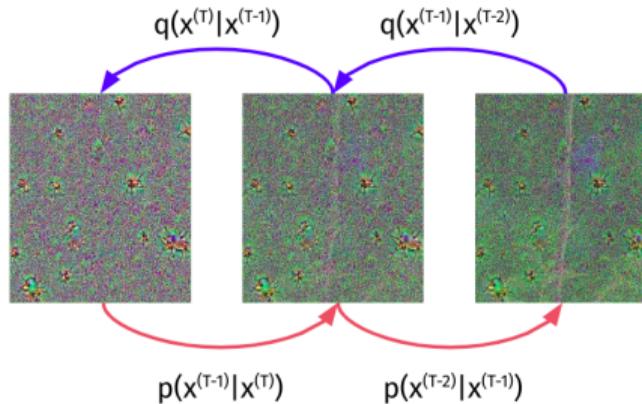
Markov property allows breaking up distributional Representation...

$$\begin{aligned} q(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T)}) &= q\left(\mathbf{x}^{(T)} \mid \mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right) q\left(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right) \\ &= q\left(\mathbf{x}^{(T)} \mid \mathbf{x}^{(T-1)}\right) q\left(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T-1)}\right) \\ &\vdots \end{aligned} \tag{1}$$

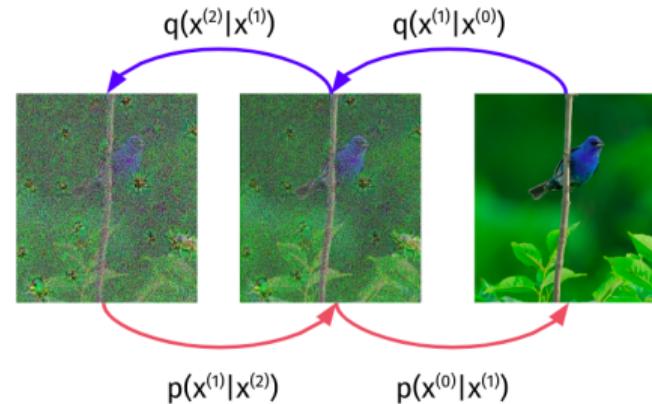
### Distributional Representation

$$q(\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T)}) = q(\mathbf{x}^{(0)}) \prod_{t=1}^T q\left(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)}\right)$$

# Reverse Diffusion Process



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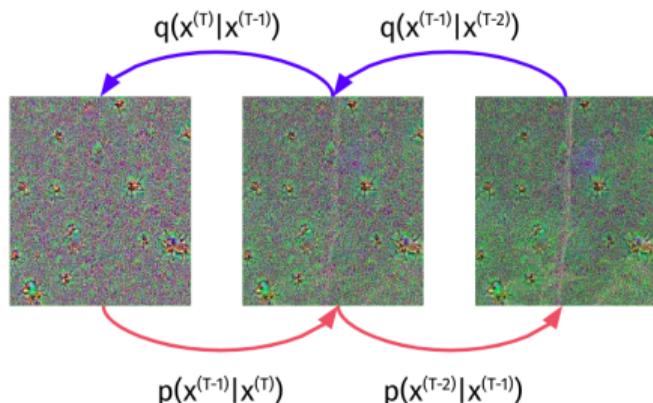


# Reverse Diffusion Process

## Fixed Forward Process

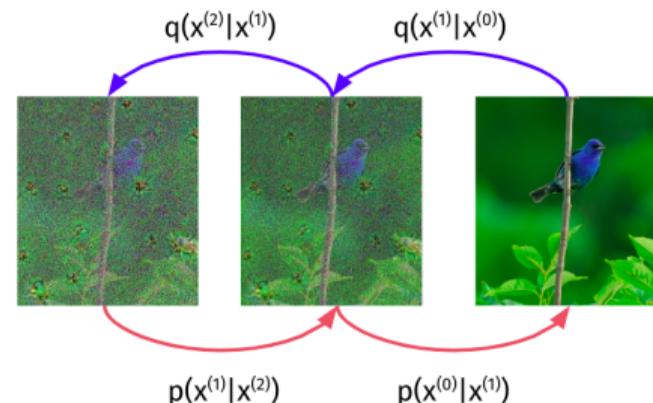
Initial Distribution

$$q(\mathbf{x}^{(0)})$$



Gaussian Transaction Kernel

$$q\left(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)}\right) = \mathcal{N}\left(\mathbf{x}^{(t)} ; \sqrt{1 - \beta_t} \mathbf{x}^{(t-1)} ; \beta_t I\right)$$

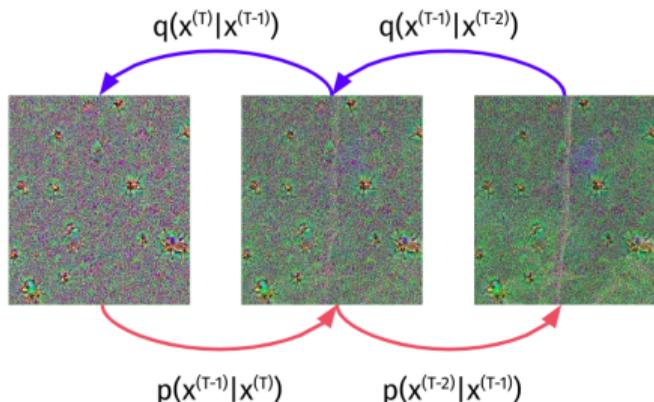


# Reverse Diffusion Process

## Fixed Forward Process

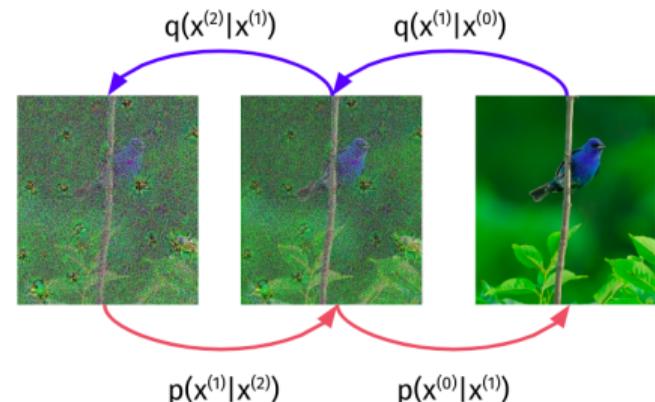
Initial Distribution

$$q(\mathbf{x}^{(0)})$$



Gaussian Transaction Kernel

$$q\left(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)}\right) = \mathcal{N}\left(\mathbf{x}^{(t)} ; \sqrt{1 - \beta_t} \mathbf{x}^{(t-1)} ; \beta_t I\right)$$



Initial Distribution

$$p(\mathbf{x}^{(T)}) \sim \mathcal{N}(0, I)$$

Approximation of

$$q(\mathbf{x}^{(t-1)} | \mathbf{x}^{(t)})$$

Gaussian Kernel with parameters

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

Learned Reverse Process

# Reverse Diffusion Process

## Forward Diffusion Process

$q(\mathbf{x}^{(0)})$  Data Distribution

$$q(\mathbf{x}^{(0\dots T)}) = q(\mathbf{x}^{(0)}) \prod_{t=1}^T q\left(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)}\right)$$

## Reverse Diffusion Process

$$q(x^{(T)}) = \mathcal{N}(0, I)$$

$$q(\mathbf{x}^{(0\dots T)}) = q(\mathbf{x}^{(T)}) \prod_{t=1}^T q\left(\mathbf{x}^{(t-1)} \mid \mathbf{x}^{(t)}\right)$$

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<sup>4</sup>Sohl-Dickstein et al., “Deep Unsupervised Learning using Nonequilibrium Thermodynamics”.

# Reverse Diffusion Process

## Forward Diffusion Process

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## Reverse Diffusion Process

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$$q(\mathbf{x}^{(0\dots T)}) = q(\mathbf{x}^{(T)}) \prod_{t=1}^T q\left(\mathbf{x}^{(t-1)} \mid \mathbf{x}^{(t)}\right)$$

Theorem. Reverse of Gaussian DP is  $\approx$  Gaussian DP<sup>4</sup>

If  $|\beta_i - \beta_{i+1}| \approx 0$ , i.e. diffusion slow enough, then

$$q(\mathbf{x}^{(t-1)} \mid \mathbf{x}^{(t)}) \approx \mathcal{N}\left(\mathbf{x}^{(t-1)}; \boldsymbol{\mu}_\theta\left(\mathbf{x}^{(t)}, t\right), \boldsymbol{\Sigma}_\theta\left(\mathbf{x}^{(t)}, t\right)\right)$$

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<sup>4</sup>Sohl-Dickstein et al., “Deep Unsupervised Learning using Nonequilibrium Thermodynamics”.

## Reverse Diffusion Process

### Forward Diffusion Process

$q(\mathbf{x}^{(0)})$  Data Distribution

$$q(\mathbf{x}^{(0\dots T)}) = q(\mathbf{x}^{(0)}) \prod_{t=1}^T q\left(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)}\right)$$

### Reverse Diffusion Process

$$q(x^{(T)}) = \mathcal{N}(0, I)$$

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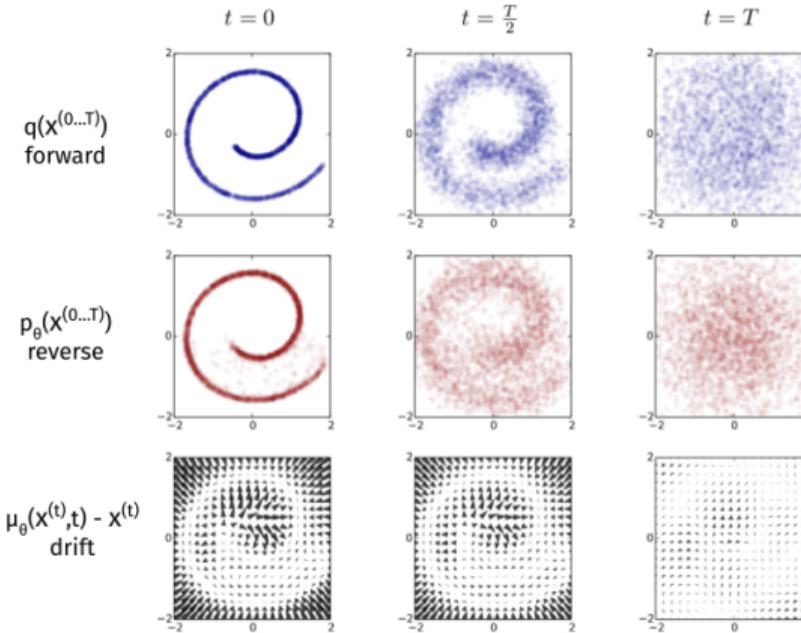
If  $|\beta_i - \beta_{i+1}| \approx 0$ , i.e. diffusion slow enough, then

$$q(\mathbf{x}^{(t-1)} \mid \mathbf{x}^{(t)}) \approx \mathcal{N}\left(\mathbf{x}^{(t-1)}; \mu_\theta(\mathbf{x}^{(t)}, t), \Sigma_\theta(\mathbf{x}^{(t)}, t)\right)$$

Mean  $\mu_\theta$  and covariance  $\Sigma_\theta$  have to be learned!!

<sup>4</sup>Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

# Visualization of Diffusion Process: 2D dimensional case



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<sup>5</sup>Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

## Training of $\mu_\theta$ and $\Sigma_\theta$

### Goal

Search for the best parameters  $\theta$

$$q(\mathbf{x}^{(0)}) \approx p_\theta(\mathbf{x}^{(0)})$$

where  $\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T)}$  diffusion process

### Estimated Reverse Process

$$p_\theta(\mathbf{x}^{(T)}) = \mathcal{N}(\mathbf{x}^{(T)}; 0, I)$$

$$p_\theta(\cdot | \mathbf{x}^{(t)}) = \mathcal{N}(\boldsymbol{\mu}_\theta(\mathbf{x}^{(t)}, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}^{(t)}, t))$$

## Training of $\mu_\theta$ and $\Sigma_\theta$

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Search for the best parameters  $\theta$

$$q(\mathbf{x}^{(0)}) \approx p_\theta(\mathbf{x}^{(0)})$$

where  $\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(T)}$  diffusion process

### Method

Minimize the Kullback–Leibler Divergence

$$D_{KL}(q || p_\theta) := \int q(\mathbf{x}^{(0)}) \log \left( \frac{q(\mathbf{x}^{(0)})}{p_\theta(\mathbf{x}^{(0)})} \right) d\mathbf{x}^{(0)}$$

### Estimated Reverse Process

$$p_\theta(\mathbf{x}^{(T)}) = \mathcal{N} \left( \mathbf{x}^{(T)}; 0, I \right)$$

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Easy??

### Estimated Reverse Process

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# Training of $\mu_\theta$ and $\Sigma_\theta$

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Easy??

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$$p_\theta(\cdot | \mathbf{x}^{(t)}) = \mathcal{N} \left( \boldsymbol{\mu}_\theta \left( \mathbf{x}^{(t)}, t \right), \boldsymbol{\Sigma}_\theta \left( \mathbf{x}^{(t)}, t \right) \right)$$

No.  $q(\mathbf{x}^{(0)})$  is  
analytically  
intractable!!



## Training of $\mu_\theta$ and $\Sigma_\theta$

Goal: Deduce a tractable loss function

$$D_{KL}(q \parallel p_\theta) := \int q(\mathbf{x}^{(0)}) \log \left( \frac{q(\mathbf{x}^{(0)})}{p_\theta(\mathbf{x}^{(0)})} \right) d\mathbf{x}^{(0)}$$

## Training of $\mu_\theta$ and $\Sigma_\theta$

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Simplification I: Minimize the Cross Entropy

$$D_{KL} \left( q(\mathbf{x}^{(0)}) \parallel p_\theta(\mathbf{x}^{(0)}) \right) = \int q(\mathbf{x}^{(0)}) \log(q(\mathbf{x}^{(0)})) d\mathbf{x}^{(0)} + \int -q(\mathbf{x}^{(0)}) \log(p_\theta(\mathbf{x}^{(0)})) d\mathbf{x}^{(0)}$$

## Training of $\mu_\theta$ and $\Sigma_\theta$

Goal: Deduce a tractable loss function

$$D_{KL}(q \parallel p_\theta) := \int q(\mathbf{x}^{(0)}) \log \left( \frac{q(\mathbf{x}^{(0)})}{p_\theta(\mathbf{x}^{(0)})} \right) d\mathbf{x}^{(0)}$$

Simplification I: Minimize the Cross Entropy

$$D_{KL} \left( q(\mathbf{x}^{(0)}) \parallel p_\theta(\mathbf{x}^{(0)}) \right) = \underbrace{\int q(\mathbf{x}^{(0)}) \log(q(\mathbf{x}^{(0)})) d\mathbf{x}^{(0)}}_{-\mathbb{H}(q(\mathbf{x}^{(0)}))} + \underbrace{\int -q(\mathbf{x}^{(0)}) \log(p_\theta(\mathbf{x}^{(0)})) d\mathbf{x}^{(0)}}_{L_{CE}(p_\theta)}$$

## Training of $\mu_\theta$ and $\Sigma_\theta$

Minimize the Cross Entropy Loss

$$L_{CE}(p_\theta(\mathbf{x}^{(0)})) := - \int q(\mathbf{x}^{(0)}) \log(p_\theta(\mathbf{x}^{(0)})) d\mathbf{x}^{(0)}$$

## Training of $\mu_\theta$ and $\Sigma_\theta$

Minimize the Cross Entropy Loss

$$L_{CE}(p_\theta(\mathbf{x}^{(0)})) := - \int q(\mathbf{x}^{(0)}) \log(p_\theta(\mathbf{x}^{(0)})) d\mathbf{x}^{(0)}$$

Observation: Marginal Distribution

$$p_\theta(\mathbf{x}^{(0)}) = \int p_\theta(\mathbf{x}^{(0\dots T)}) d\mathbf{x}^{(1\dots T)}$$

## Training of $\mu_\theta$ and $\Sigma_\theta$

Minimize the Cross Entropy Loss

$$L_{CE}(p_\theta(\mathbf{x}^{(0)})) := - \int q(\mathbf{x}^{(0)}) \log(p_\theta(\mathbf{x}^{(0)})) d\mathbf{x}^{(0)}$$

Observation: Marginal Distribution

$$p_\theta(\mathbf{x}^{(0)}) = \int p_\theta(\mathbf{x}^{(0\dots T)}) d\mathbf{x}^{(1\dots T)}$$

Simplification II: Jensen Inequality

$$L_{CE}(p_\theta) \leq -\mathbb{E}_{q(\mathbf{x}^{(0\dots T)})} \left[ \log \frac{q(\mathbf{x}^{(1\dots T)} | \mathbf{x}^{(0)})}{p_\theta(\mathbf{x}^{(0\dots T)})} \right]$$

## Training of $\mu_\theta$ and $\Sigma_\theta$

...after some algebraic steps :)

### Reformulated Loss Function

$$\mathcal{L} = \mathcal{L}_T + \sum_{t=1}^{T-1} \mathcal{L}_t + \mathcal{L}_0$$

where,

$$\mathcal{L}_T = \mathbb{E}_{q(\mathbf{x}^{(0\dots T)})} \left[ D_{KL} \left( q(\mathbf{x}^{(T)} | \mathbf{x}^{(0)}) \parallel p_\theta(\mathbf{x}^{(T)}) \right) \right]$$

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}^{(0\dots T)})} \left[ D_{KL} \left( q(\mathbf{x}^{(t)} | \mathbf{x}^{(t+1)}, \mathbf{x}^{(0)}) \parallel p_\theta(\mathbf{x}^{(t)} | \mathbf{x}^{(t+1)}) \right) \right]$$

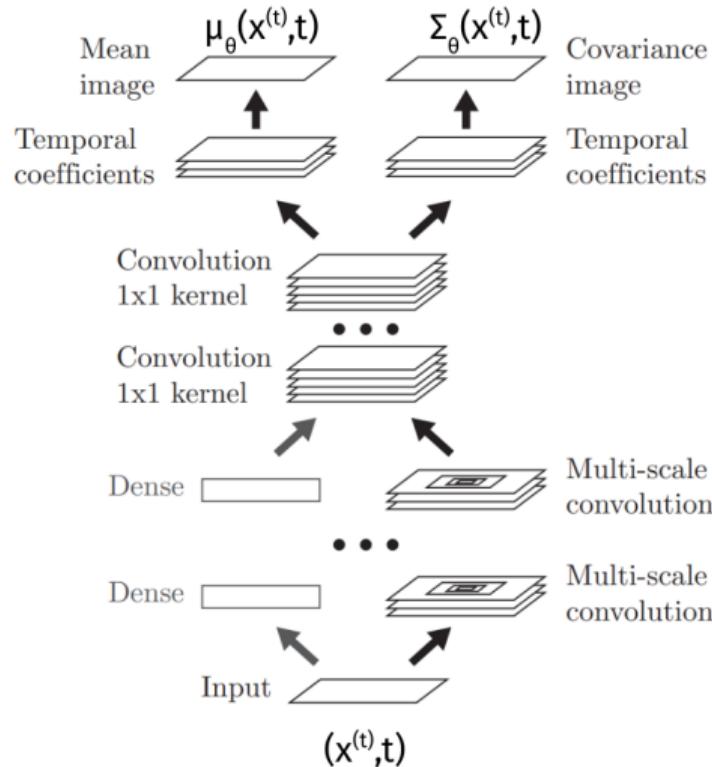
$$\mathcal{L}_0 = \mathbb{E}_{q(\mathbf{x}^{(0\dots T)})} \left[ p_\theta(\mathbf{x}^{(0)} | \mathbf{x}^{(1)}) \right]$$

Note.

$\mathcal{L}_T$  is constant.

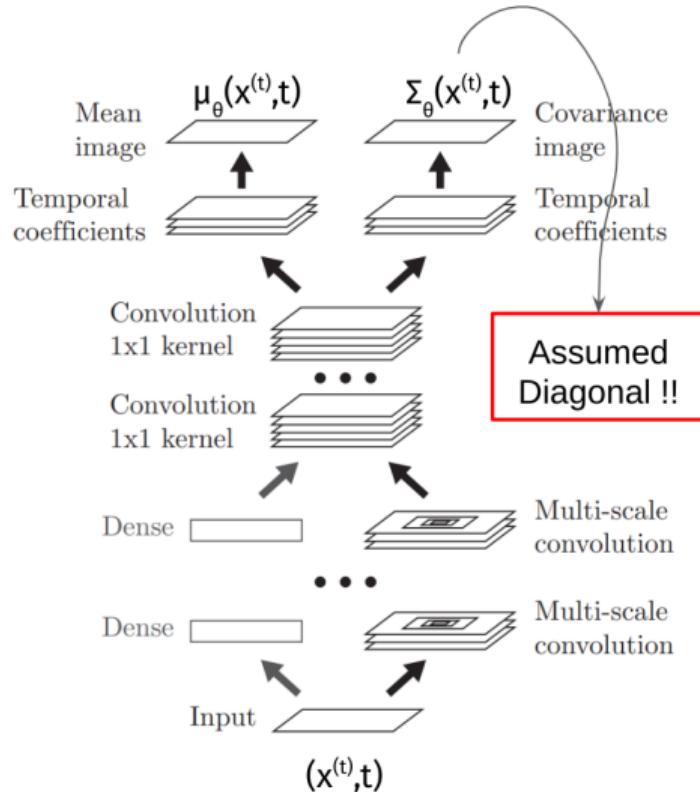
$\mathcal{L}_0, \mathcal{L}_t$  explicit.

## Neural Network that estimate $\mu_\theta$ and $\Sigma_\theta$



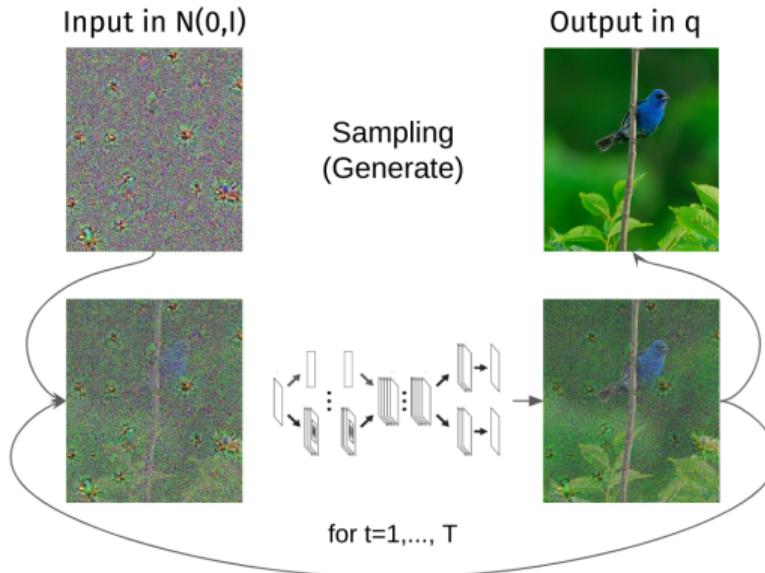
Proposed Neural Network for CIFAR10 image generation. T=1000

# Neural Network that estimate $\mu_\theta$ and $\Sigma_\theta$



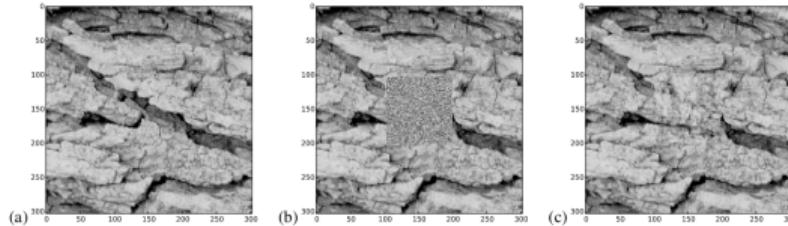
Proposed Neural Network for CIFAR10 image generation. T=1000

## Sampling or Generative Stage



# Experiments<sup>6</sup>

Bark Dataset



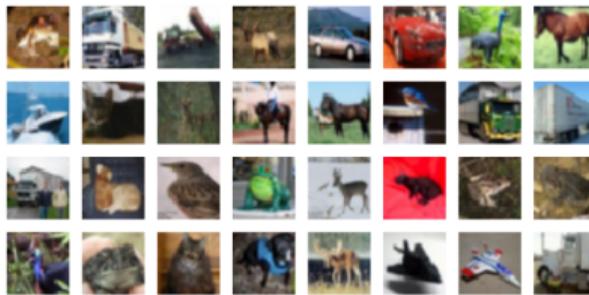
MNIST

3	4	2	1	8	6	7	7	8	7
5	5	3	2	6	7	0	4	8	2
8	8	2	8	9	1	6	8	E	4
0	2	0	7	4	9	5	4	2	7
8	2	1	9	3	6	5	0	6	0
E	7	4	4	5	2	6	9	3	3
7	6	4	6	9	4	1	0	2	9
7	0	0	1	7	7	4	2	0	1
7	4	3	0	5	2	6	2	6	4
1	8	9	9	8	9	1	3	5	4

<sup>6</sup>Sohl-Dickstein et al., “Deep Unsupervised Learning using Nonequilibrium Thermodynamics”.

# Experiments<sup>7</sup>

CIFAR10 (original)



CIFAR10 (generated)



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<sup>7</sup>Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

## Timeline

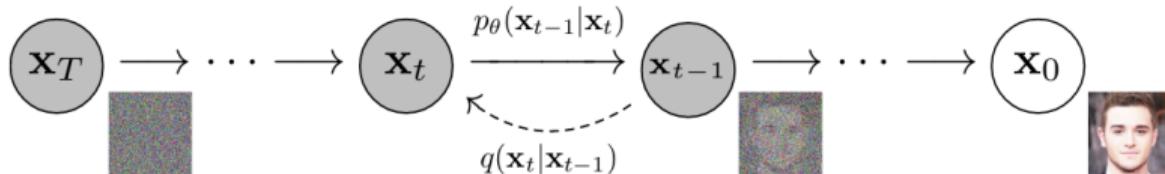
2015) ...*Non-equilibrium Thermodynamics*. Sohl-Dickstein et al. ICML. ✓

2020) *Denoising Diffusion Probabilistic Models*. Ho et al. NeurIPS.

2021) *Score-Based Generative Modeling Through SDE*. Song et al. ICLR.

# Denoising Diffusion Probabilistic Model

Small technical improvements highly impact the performance...<sup>8</sup>



## Simplification I: Diagonal Uniform Covariance Matrix

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

where

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

<sup>8</sup>Ho, Jain, and Abbeel, "Denoising Diffusion Probabilistic Models".

Previous work aims at estimating  $\mu_\theta(\mathbf{x}^{(t)}, t)$  and  $\Sigma_\theta(\mathbf{x}^{(t)}, t)$ .

## Simplification II: Estimating the committed error

$$\mu_\theta(\mathbf{x}^{(t)}) = \frac{1}{\sqrt{1 - \beta_t}} \left( \mathbf{x}^{(t)} - \frac{1 - \beta_t}{\sqrt{\alpha_t}} \varepsilon_\theta(\mathbf{x}^{(t)}, t) \right)$$

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$\epsilon_\theta(\mathbf{x}^{(t)}, t)$  DNN (U-Net) with learnable parameters!!

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$\varepsilon_\theta(\mathbf{x}^{(t)}, t)$  DNN (U-Net) with learnable parameters!!

Simplification III: Training on random instants  $t$

$$\mathcal{L}_{simple} = \mathbb{E}_{t, \mathbf{x}^{(0)}, \varepsilon} \left[ \left\| \varepsilon - \varepsilon_\theta \left( \sqrt{1-\alpha_t} \mathbf{x}^{(0)} + \sqrt{\alpha_t} \varepsilon, t \right) \right\| \right]$$

where

$$t \sim \mathcal{U}\{1, \dots, T\}, \quad \mathbf{x}^{(0)} \sim q, \quad \varepsilon \sim \mathcal{N}(0, I)$$

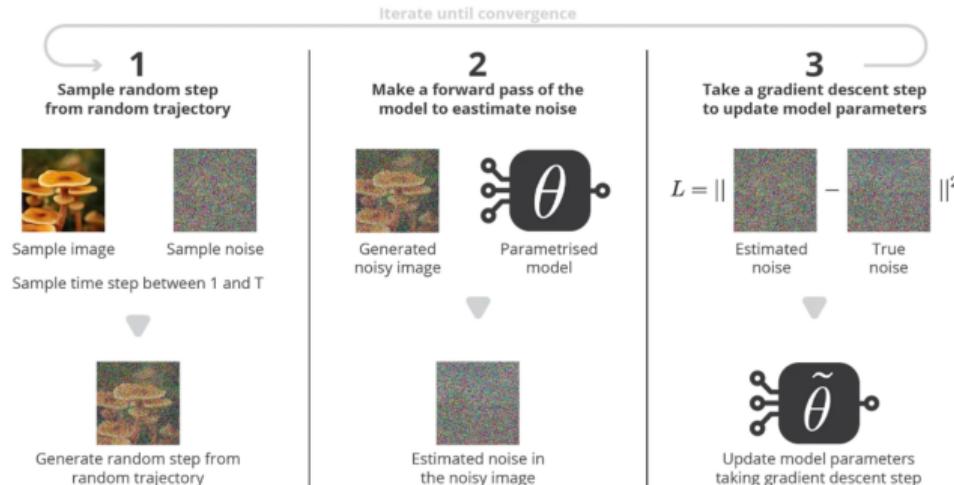
# Training and Sampling Procedure

## 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
        $\nabla_{\theta} \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t)\|^2$ 
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:    $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \alpha_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$ 
5: end for
6: return  $\mathbf{x}_0$ 
```



# Experiments: Sample Quality

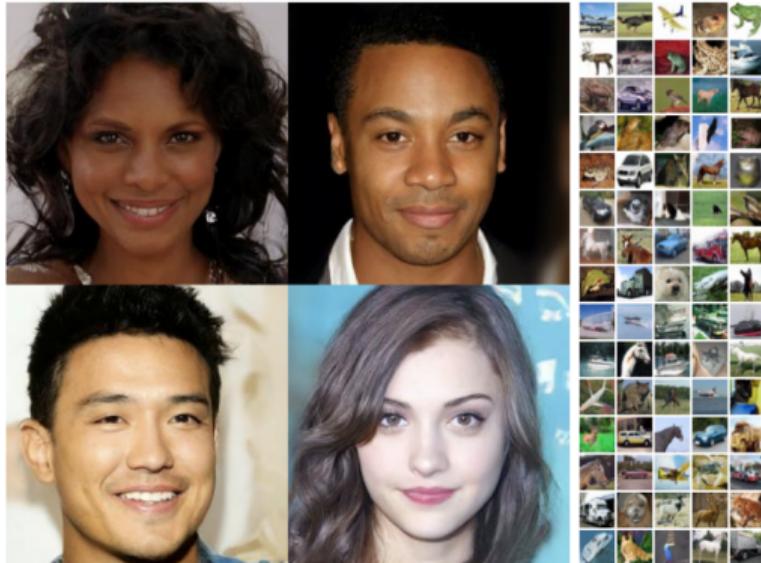


Figure 1: Generated samples on CelebA-HQ  $256 \times 256$  (left) and unconditional CIFAR10 (right)

Objective	IS	FID
<b><math>\tilde{\mu}</math> prediction (baseline)</b>		
$L$ , learned diagonal $\Sigma$	$7.28 \pm 0.10$	23.69
$L$ , fixed isotropic $\Sigma$	$8.06 \pm 0.09$	13.22
$\ \tilde{\mu} - \tilde{\mu}_\theta\ ^2$	-	-
<b><math>\epsilon</math> prediction (ours)</b>		
$L$ , learned diagonal $\Sigma$	-	-
$L$ , fixed isotropic $\Sigma$	$7.67 \pm 0.13$	13.51
$\ \tilde{\epsilon} - \epsilon_\theta\ ^2$ ( $L_{\text{simple}}$ )	<b><math>9.46 \pm 0.11</math></b>	<b>3.17</b>

Metrics for CIFAR10

Note.

1. Low FID (Frechet Implicit Distance)  $\Rightarrow$  high quality
2. Training improved

# Experiments: Diffusion vs GAN/VAE

*“Diffusion models get comparable result to Generative Adversarial Networks and Variational Autoencoders”*

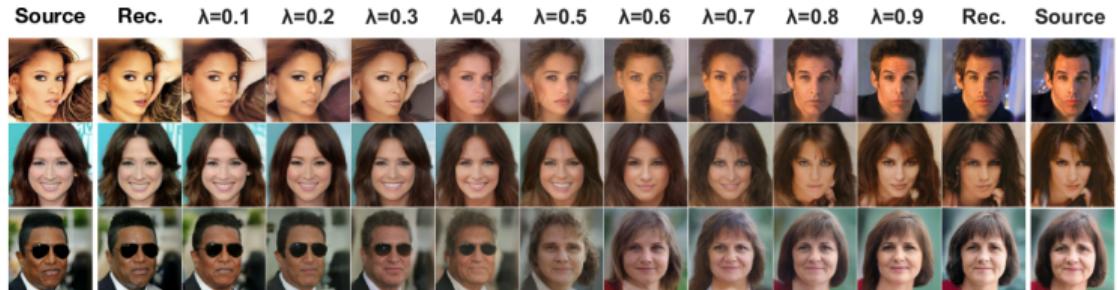
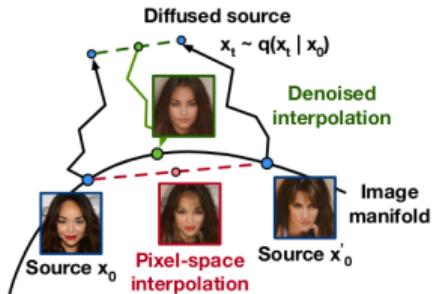
Table 1: CIFAR10 results. NLL measured in bits/dim.

Model	IS	FID	NLL Test (Train)
<b>Conditional</b>			
EBM [4]	8.30	37.9	
JEM [2]	8.76	38.4	
BigGAN [3]	9.22	14.73	
StyleGAN2 + ADA (v1) [20]	<b>10.06</b>	<b>2.67</b>	
<b>Unconditional</b>			
Diffusion (original) [53]			$\leq 5.40$
Gated PixelCNN [59]	4.60	65.93	3.03 (2.90)
Sparse Transformer [2]			<b>2.80</b>
PixelCNN [44]	5.29	49.46	
EBM [4]	6.78	38.2	
NCSNv2 [56]			31.75
NCSN [53]	$8.87 \pm 0.12$	25.32	
SNGAN [39]	$8.22 \pm 0.05$	21.7	
SNGAN-DDLS [4]	$9.09 \pm 0.10$	15.42	
StyleGAN2 + ADA (v1) [20]	<b><math>9.74 \pm 0.05</math></b>	3.26	
Ours ( $L$ , fixed isotropic $\Sigma$ )	$7.67 \pm 0.13$	13.51	$\leq 3.70$ (3.69)
<b>Ours (<math>L_{\text{simple}}</math>)</b>	$9.46 \pm 0.11$	<b>3.17</b>	$\leq 3.75$ (3.72)

CIFAR10 results. NLL measured in bits/dim<sup>10</sup>

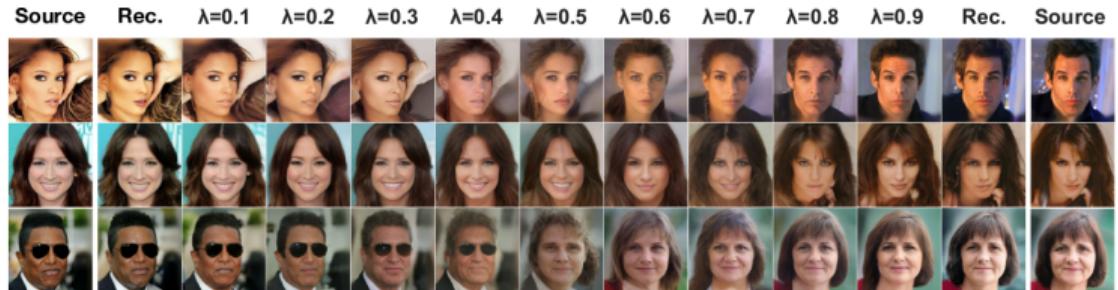
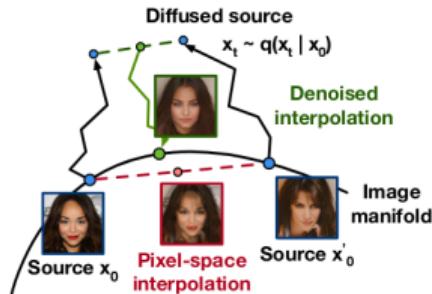
<sup>10</sup>Ho, Jain, and Abbeel, “Denoising Diffusion Probabilistic Models”.

# Experiments: Images Interpolation



$$\mathbf{x}_\lambda^{(T)} := \lambda \mathbf{x}_{\text{source}_r}^{(T)} + (1 - \lambda) \mathbf{x}_{\text{source}_l}^{(T)}, \quad \lambda \in [0, 1]$$

# Experiments: Images Interpolation



$$\mathbf{x}_\lambda^{(T)} := \lambda \mathbf{x}_{\text{source}_r}^{(T)} + (1 - \lambda) \mathbf{x}_{\text{source}_l}^{(T)}, \quad \lambda \in [0, 1]$$

$$\mathbf{x}_\lambda^{(0)} \sim p_\theta(\mathbf{x}^{(T)}), \quad \text{by diffusion}$$

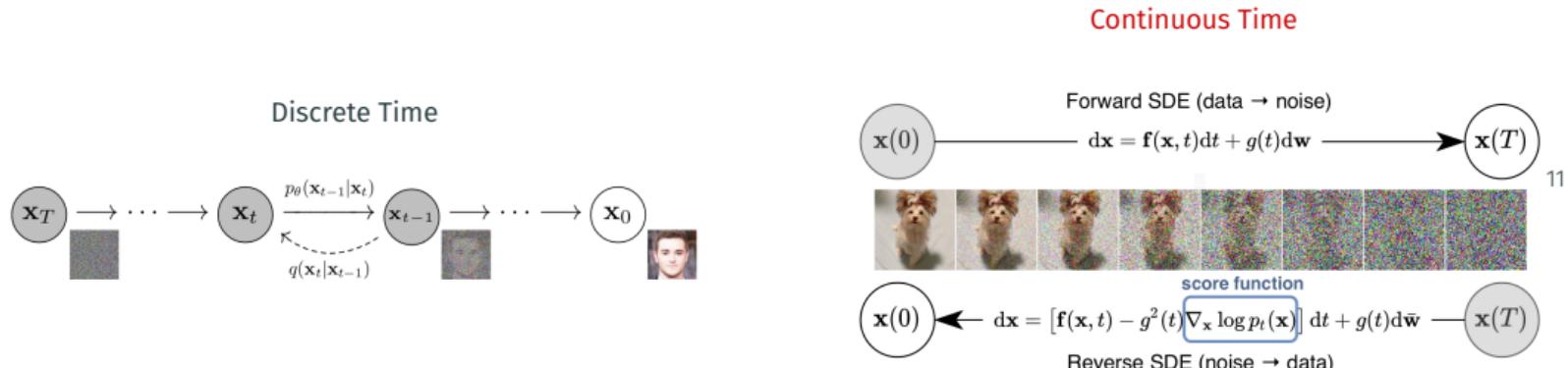
## Timeline

2015) ...*Non-equilibrium Thermodynamics*. Sohl-Dickstein et al. ICML. ✓

2020) *Denoising Diffusion Probabilistic Models*. Ho et al. NeurIPS.✓

2021) *Score-Based Generative Modeling Through SDE*. Song et al. ICLR.

# Score-Based Generative Modeling Through SDE (no details)



## Stochastic Process

Continuous sequence of  $\mathbf{x}$  indexed by  $t \in [0, T]$ , where  $\mathbf{x}(t)$  has distribution  $p_t(\mathbf{x})$ ;

<sup>11</sup>Song et al., "Score-based generative modeling through stochastic differential equations".

# Continuous Diffusion Process described by SDE

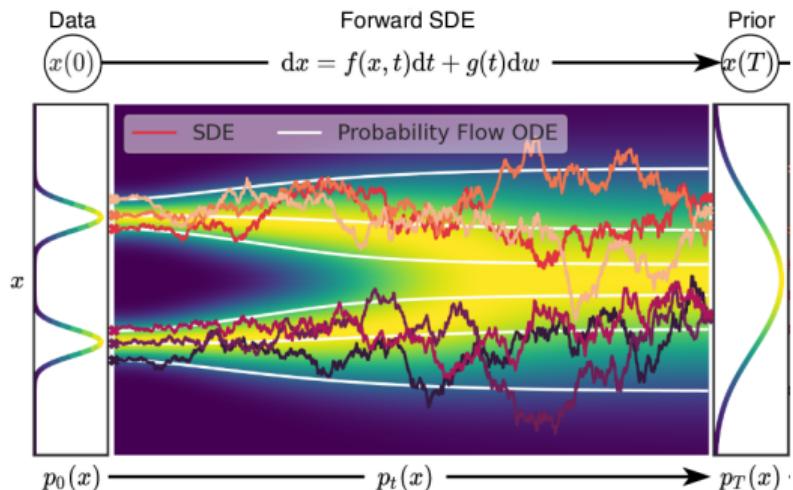
## Continuous Diffusion Process

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

1.  $f(\mathbf{x}, t)$  drift coefficient.
2.  $g(t)$  diffusion coefficient.
3.  $\mathbf{w}(t)$ , Weiner Process

## Weiner Process

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t-s)I)$$



# Reverse Process explicity given by $\nabla_x p_t(\mathbf{x})$

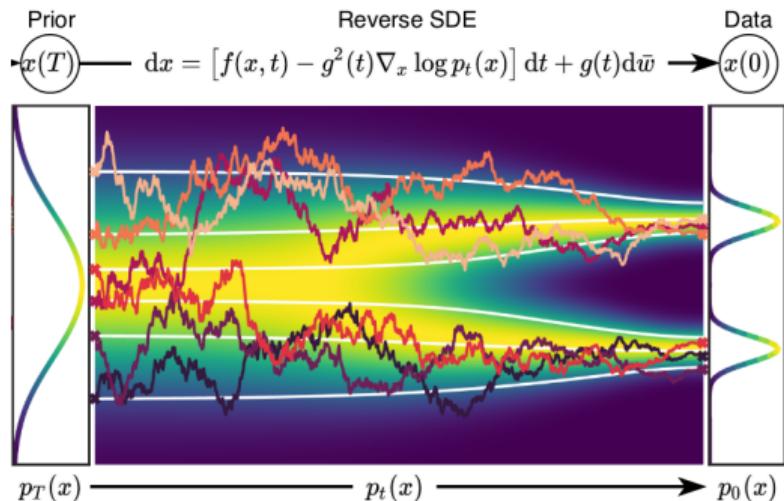
## Theorem

Reverse Process is still a diffusion process

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

where

- $\bar{f}(\mathbf{x}, t) = f(\mathbf{x}, t) - g(t)^2 \nabla_{\mathbf{x}} \log(p_t(\mathbf{x}))$
- $\bar{\mathbf{w}}(t) = \mathbf{w}(T - t)$ , reverse Weiner Process



DALL-E2

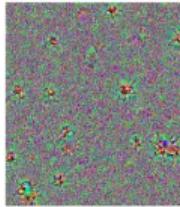
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# Introduction

A Ramesh et al. (Open AI). “*Hierarchical Text-Conditional Image Generation with CLIP Latents*.”. February 2022.

From an analytic distribution to image distribution



Unconditional  
Generative Model



<sos>A Blue-and-black tanager hanging on a branch looking forward to the left with a green background .<eos>

Text-Conditioned  
Generative Model



From a distribution in the a latent space  
to image distribution



vibrant portrait painting of Salvador Dalí with a robotic half face

a shiba inu wearing a beret and black turtleneck



an espresso machine that makes coffee from human souls, artstation

panda mad scientist mixing sparkling chemicals, artstation

# Introduction

DALL-E2: a new AI system that can create realistic images and art from a description in natural language

An astronaut Teddy bears A bowl of soup

mixing sparkling chemicals as mad scientists shopping for groceries working on new AI research

as a 1990s Saturday morning cartoon as digital art in a steampunk style



12

---

<sup>12</sup>Credits: DALL-E2 website

# Introduction

DALL-E2: a new AI system that can create realistic images and art from a description in natural language

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



12

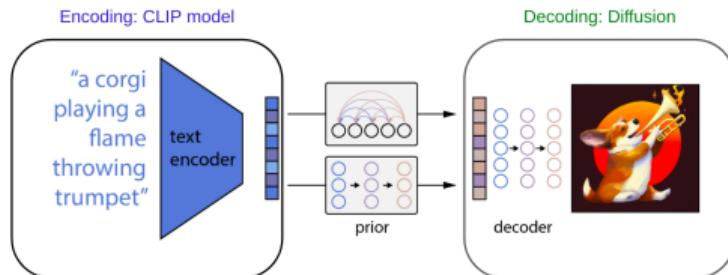
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<sup>12</sup>Credits: DALL-E2 website

# Overview: CLIP + Diffusion

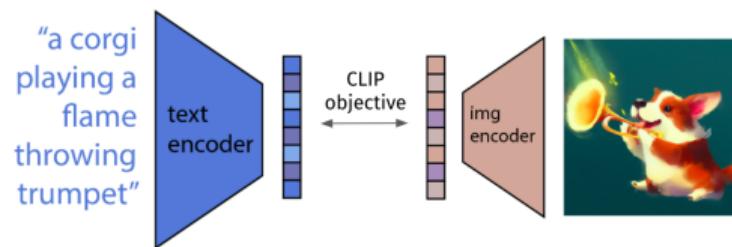
13

## Text-to-Image Generation with CLIP



Diffusion models allows generating images with high sample fidelity and photorealism

## CLIP model

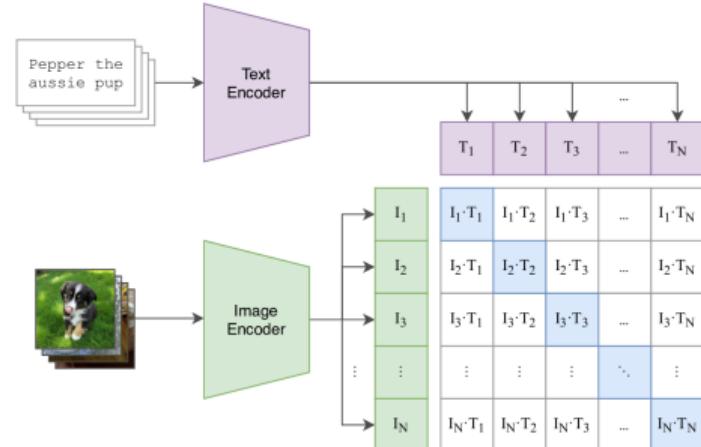


Embedding of images and text in the same latent space

<sup>13</sup>Ramesh et al., "Hierarchical Text-Conditional Image Generation with CLIP Latents".

# CLIP: Latent Embedding model

1. The **Text Encoder** takes as input a text  $y$  in and embeds it in  $z \in \mathbb{R}^n$ .
2. The **Image Encoder** takes as input an image  $x$  and embeds it in the latent space  $\mathbb{R}^n$ .
3. **Property:** The two embedded objects can be directly compared through cosine similarity.

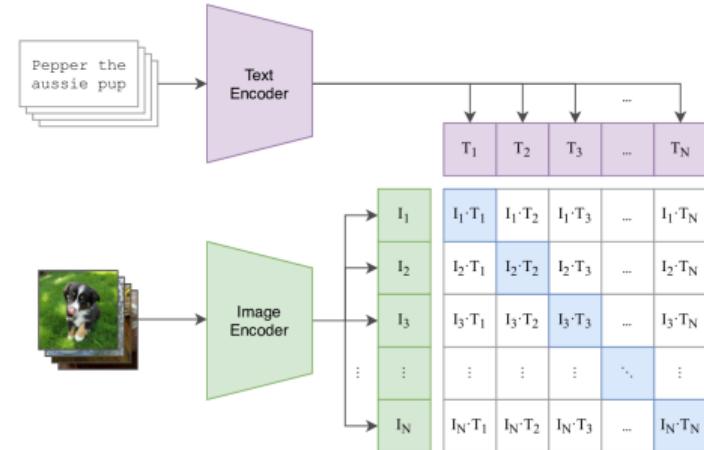


CLIP allows embedding of images and text in the same latent space.

<sup>14</sup> Radford et al., "Learning Transferable Visual Models From Natural Language Supervision".

# CLIP: Latent Embedding model

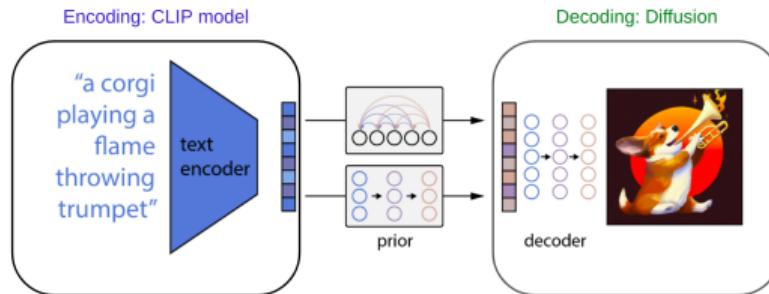
4. Aim: Zero-shot classification (of unseen datasets, see later.)
5. The Text Encoder is a Transformer for NLP (63M of parameters, next lectures).
6. The Image Encoder include ResNet-50 and Vision-Transformers



CLIP allows embedding of images and text in the same latent space.

<sup>14</sup> Radford et al., “Learning Transferable Visual Models From Natural Language Supervision”.

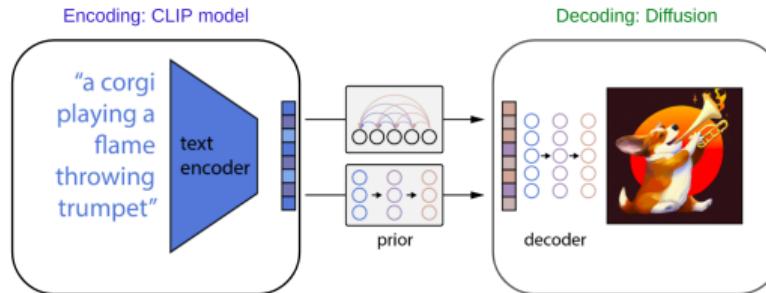
## DALL-E2 with higher detail



Let  $(x, y)$  be an (image, caption) pair.

1. CLIP such that  $(x, y) \mapsto (z_i, z_t)$ .
2. Prior which estimates  $q(z_i | y)$
3. Decoder which estimate  $q(x | z_i, y)$

## DALL-E2 with higher detail

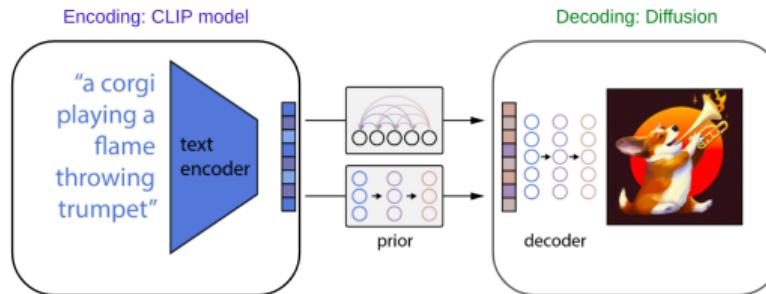


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*Provide an image embedding conditioned to a text.  
Provide an Image conditioned to a text and Image Emb.*

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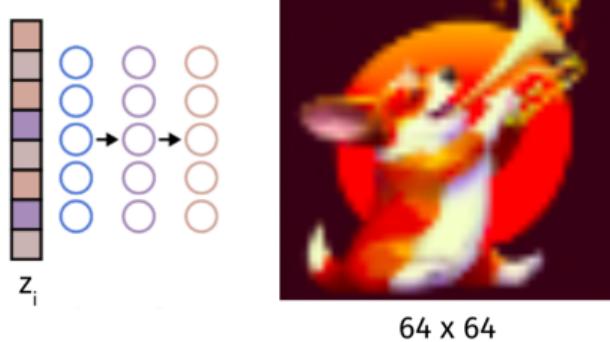
## Observation

$$p(x | y) \underset{\text{Deterministic}}{=} p(x, z_i | y) \underset{\text{Bayes Rule}}{=} p(x | z_i, y)p(z_i | y)$$

## Decoding through Diffusion models

Step 1: Generate a low-resolution image from  $z_i$

A guided diffusion model is used to get a low resolution image from the image embedding.



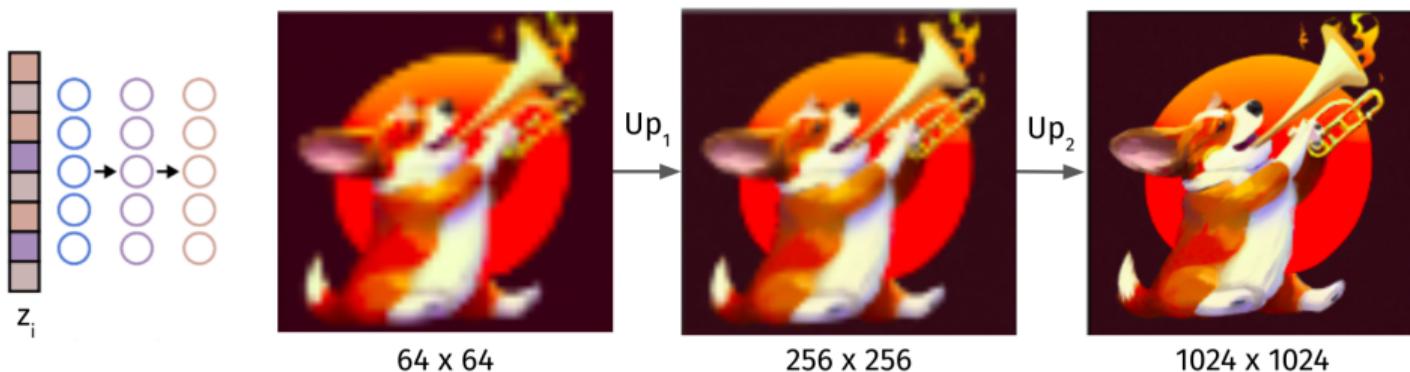
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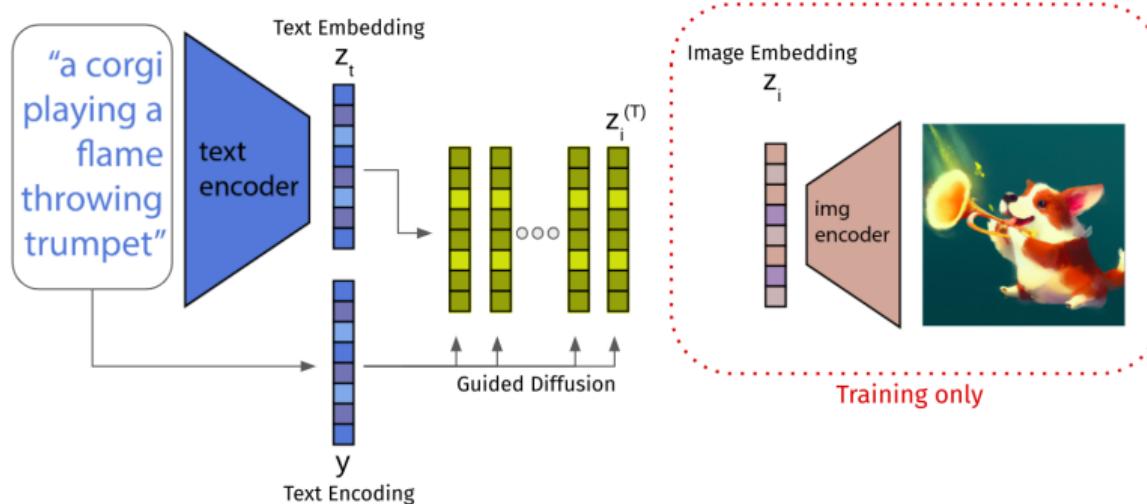
Step 2. Upsampling Procedure

Two diffusion models are used to increase the resolution of the image from low to super-high



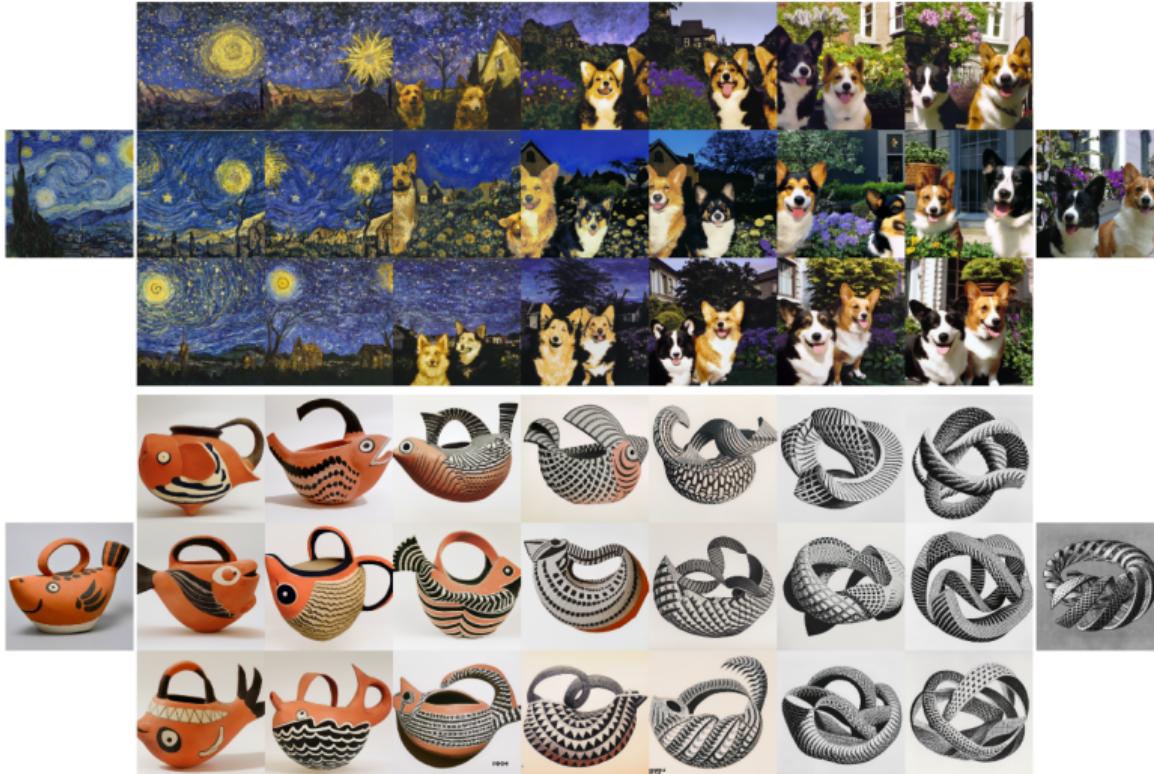
## Prior

Diffusion Prior: “The image embedding  $\mathbf{z}_i$  is directly modelled using a Gaussian diffusion model conditioned on the caption  $\mathbf{y}$ ”.



$$\text{Training Loss Function } L_{prior} = \mathbb{E}_{t \sim [1, T], \mathbf{z}_i^{(t)} \sim q_t} \left[ \|f_\theta(\mathbf{z}_i^{(t)}, \mathbf{y}, t) - \mathbf{z}_i\|^2 \right] \quad \text{where } \mathbf{z}_i^{(0)} = \mathbf{z}_t$$

## Experiments: Image Interpolation



For each row, the decoder is applied to a combination of  $\mathbf{z}_i(\text{left})$  and  $\mathbf{z}_i(\text{right})$ .

### Representation of the Dignity

## Experiments: Abstract Representation

Representation of the Dignity



DALL-E2

## Experiments: Abstract Representation

Representation of the Dignity



DALL-E2



Matt Groening (S8 E6)

# Experiments: Recreate Ancient Works



Benjamin Hilton  
@benjamin\_hilton · [Follow](#)



Got access to DALL-E - here, have a medieval painting of the wifi not working



10:45 PM · Apr 27, 2022



Lapine  
@LapineDeLaTerre · [Follow](#)



An ancient Egyptian painting depicting an argument over whose turn it is to take out the trash #dalle



10:23 AM · Apr 24, 2022



## Conclusion

---



1. Diffusion models, as generative models, can be used for malicious porpose. Fake images can become less detectable.
2. Diffusion models reflects the biases in the dataset with which they are trained. Hence, using generated images for training other models can produce a **fade-in** effect.

---

<sup>15</sup>Ho, Jain, and Abbeel, “Denoising Diffusion Probabilistic Models”.

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2. Diffusion models reflects the biases in the dataset with which they are trained. Hence, using generated images for training other models can produce a **fade-in effect**.

*“If samples from generative models trained on these datasets proliferate throughout the internet, then these biases will only be reinforced further.<sup>15</sup>”*

---

<sup>15</sup> Ho, Jain, and Abbeel, “Denoising Diffusion Probabilistic Models”.

1. Diffusion Generative Models (from 2015 to 2022)
2. Overview on CLIP model for representation learning.
3. The Diffusion models inside DALL-E2

# Thanks for the attention

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*Retis*  
Real-Time Systems Laboratory

## Proof Details

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## Proof of Explicit Representation of Forward Diffusion Process

Let us proceeding by induction by assuming  $\mathbf{x}^{(t)} = \sqrt{1 - \alpha_t} \mathbf{x}^{(0)} + \sqrt{\alpha_t} \boldsymbol{\varepsilon}$  where  $\boldsymbol{\varepsilon} \sim \mathcal{N}(0, I)$  and where  $\alpha_t = 1 - \prod_{i=0}^t (1 - \beta_i)$ .

$$\begin{aligned}\mathbf{x}^{(t+1)} &= \sqrt{1 - \beta_{t+1}} \mathbf{x}^{(t)} + \sqrt{\beta_{t+1}} \boldsymbol{\varepsilon}_{t+1} \\ &= \sqrt{1 - \beta_{t+1}} \left( \sqrt{1 - \alpha_t} \mathbf{x}^{(0)} + \sqrt{\alpha_t} \boldsymbol{\varepsilon} \right) + \sqrt{\beta_{t+1}} \boldsymbol{\varepsilon}_{t+1} \\ &= \sqrt{\left( \prod_{i=0}^{t+1} (1 - \beta_i) \right)} \mathbf{x}^{(0)} + \sqrt{(1 - \beta_{t+1})\alpha_t + \beta_{t+1}} \tilde{\boldsymbol{\varepsilon}}\end{aligned}\tag{2}$$

where the last term of the summation is obtained by observing that, since  $\sqrt{(1 - \beta_{t+1})\alpha_t} \boldsymbol{\varepsilon}$  and  $\sqrt{\beta_{t+1}} \boldsymbol{\varepsilon}_{t+1}$  are independent, then the variance of their sum (that still has a gaussian distribution) is given by  $(1 - \beta_{t+1})\alpha_t + \beta_{t+1}$ .

