

Diffusion Models and an application to DALL-E2

Deep Learning and Neural Networks: Advanced Topics

Fabio Brau

March 1, 2023

Scuola Superiore Sant'Anna, Pisa.

TELECOMMUNICATIONS,
COMPUTER
ENGINEERING,
AND PHOTONICS
INSTITUTE



Sant'Anna
School of Advanced Studies – Pisa



Introduction

Diffusion Models

DALL-E2

Conclusion

Introduction



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*

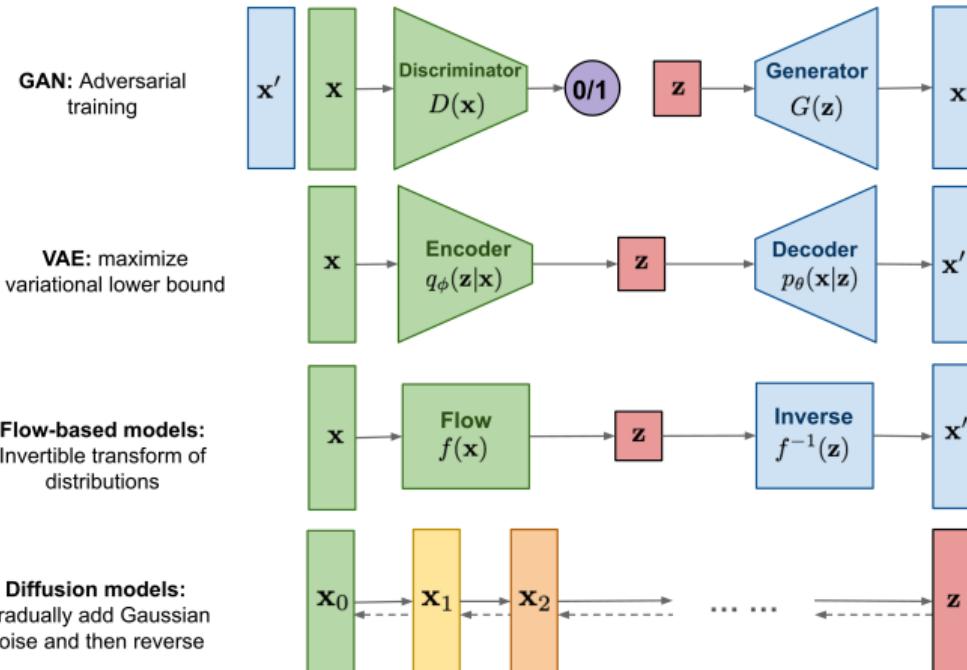
*High dimension data
point from simple
noise distribution*

*High dimension data
point from complex
image distribution*

Schema of generative models¹

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

Generative Models



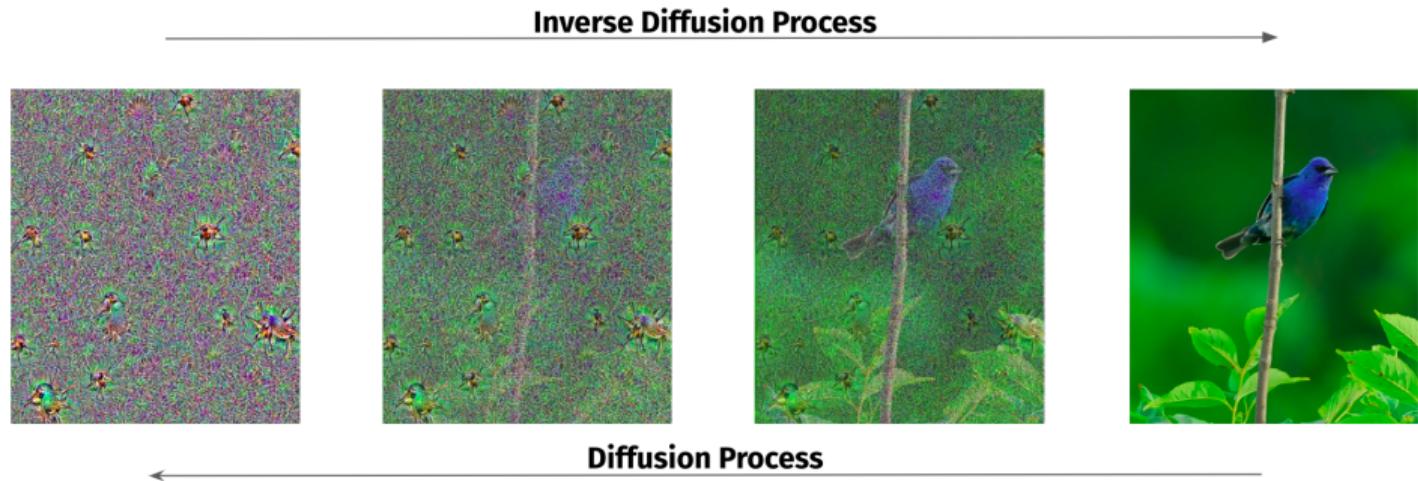
Overview of different generative models²

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

Diffusion Models



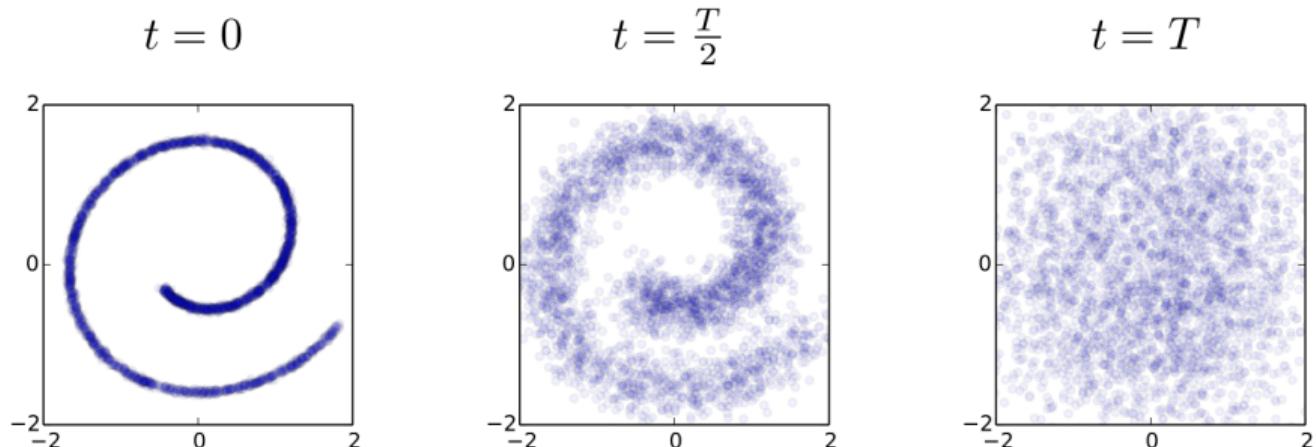
Diffusion models are generative models that aim at denoising data



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.³

³Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

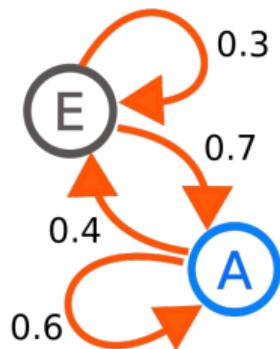
Reminder: Markov Chains with Discrete Time

Informal Definition

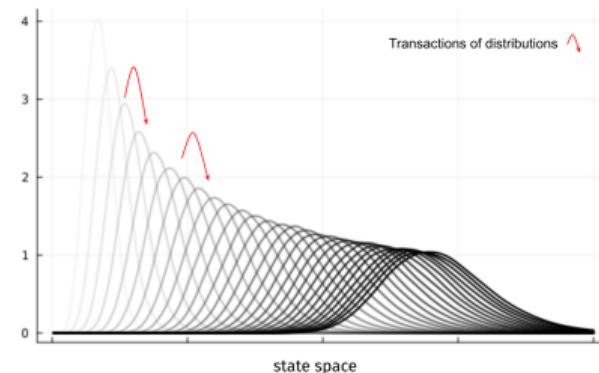
A sequence of random variables $x^{(0)}, x^{(1)}, \dots, x^{(t)}, \dots$, such that

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

Reminder: Discrete Time Markov Chain with Discrete State Space

Definition

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

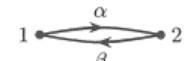
P is a stochastic matrix!

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

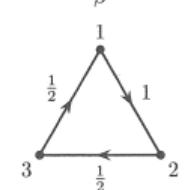
- Discrete state space: $S = \{s_0, \dots, s_n, \dots\}$

- 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 $p(\mathbf{x} \mid \mathbf{y})$

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

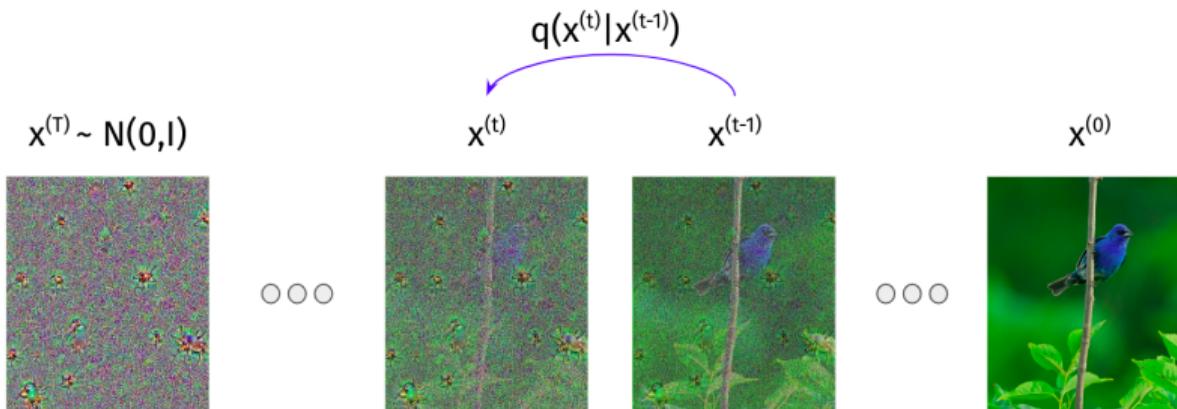
Marginal Distribution $p(\mathbf{x})$

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

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: $0 < \beta_1 < \dots < \beta_T < 1$

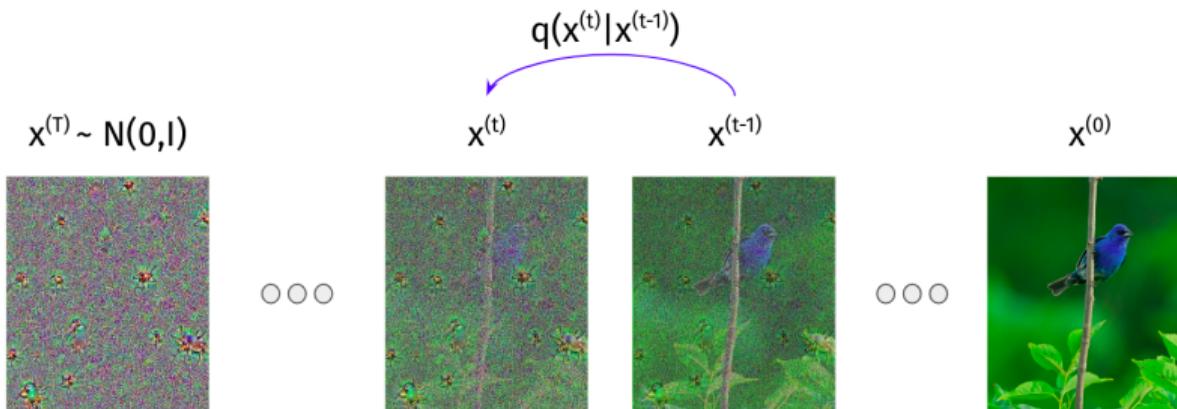


Forward Diffusion Process

“Adding noise to data...”

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

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: Distribution Representation

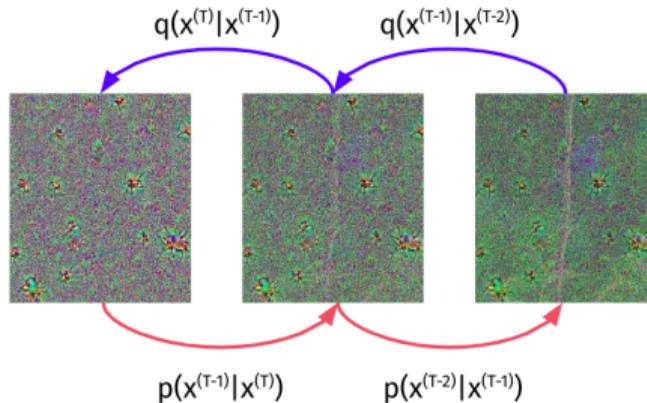
Markov property allows breaking up distributional Representation...

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

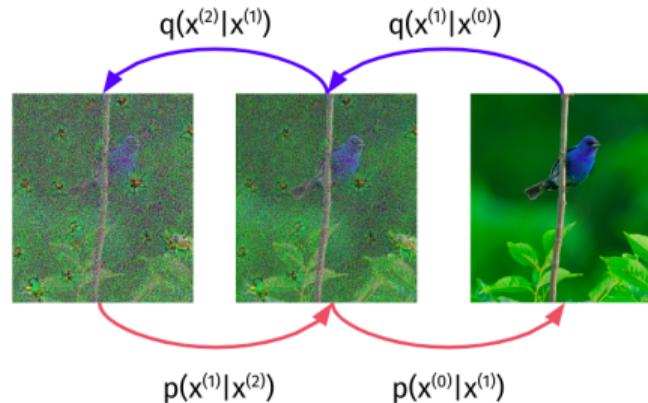
Distributional Representation

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

Reverse Diffusion Process



○ ○ ○

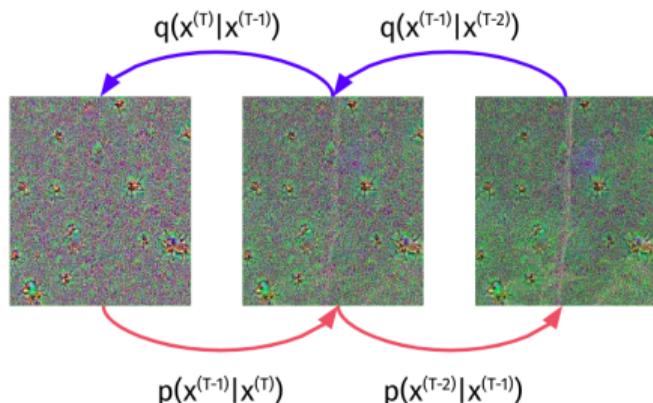


Reverse Diffusion Process

Fixed Forward Process

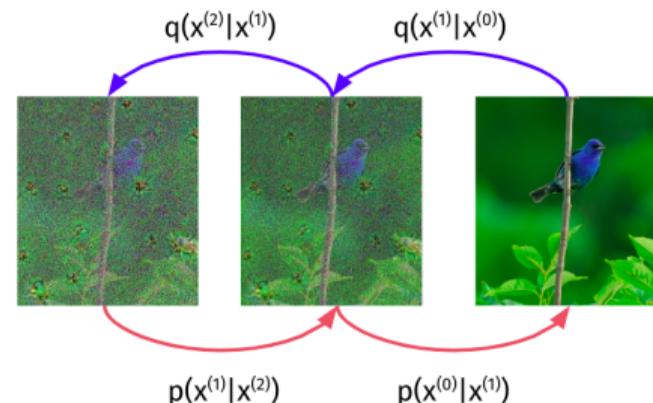
Initial Distribution

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



Gaussian Transaction Kernel

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

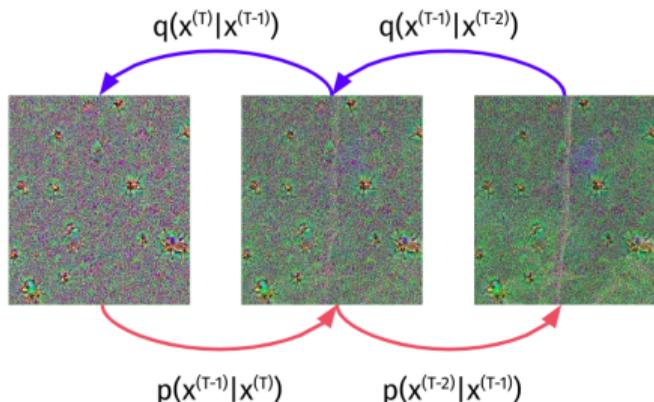


Reverse Diffusion Process

Fixed Forward Process

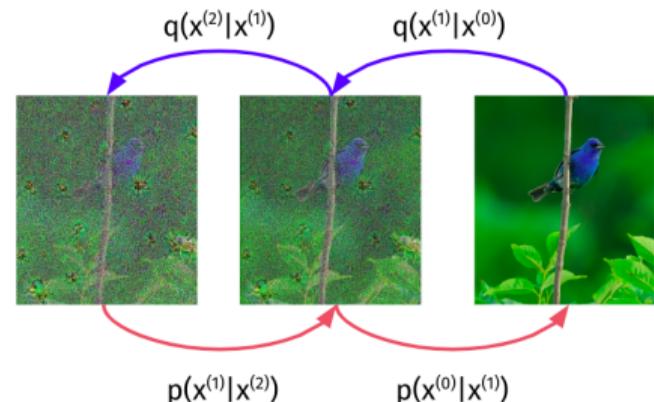
Initial Distribution

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



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

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

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

⁴Sohl-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

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

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

Theorem. Reverse of Gaussian DP is \approx Gaussian DP⁴

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

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

⁴Sohl-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

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

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

Theorem. Reverse of Gaussian DP is \approx Gaussian DP⁴

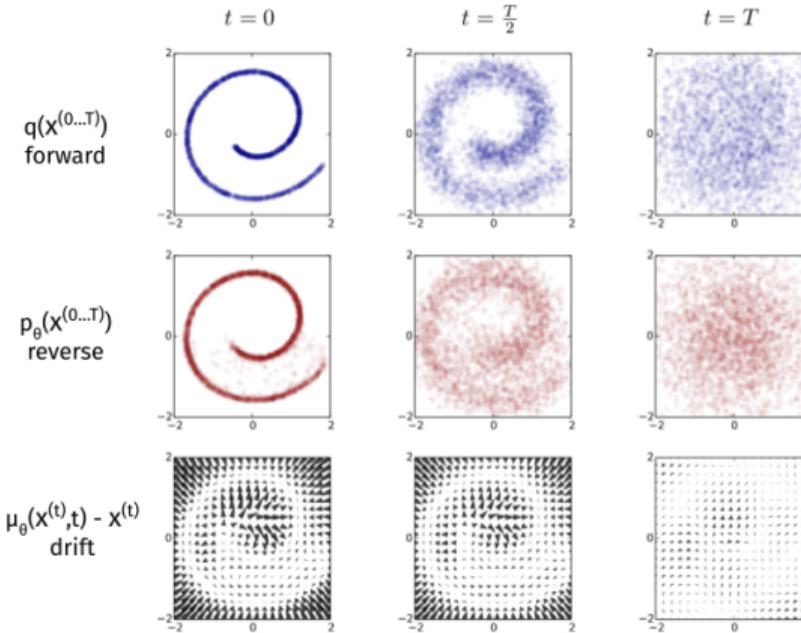
If $|\beta_i - \beta_{i+1}| \approx 0$, i.e. diffusion slow enough, then

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

Mean $\boldsymbol{\mu}_\theta$ and covariance $\boldsymbol{\Sigma}_\theta$ have to be learned!!

⁴Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

Visualization of Diffusion Process: 2D dimensional case



5

⁵Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

Training of μ_θ and Σ_θ

Goal

Search for the best parameters θ

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

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 μ_θ and Σ_θ

Goal

Search for the best parameters θ

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

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

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

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

Training of μ_θ and Σ_θ

Goal

Search for the best parameters θ

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

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

Method

Minimize the Kullback–Leibler Divergence

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

Easy??

Estimated Reverse Process

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

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

Training of μ_θ and Σ_θ

Goal

Search for the best parameters θ

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

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

Method

Minimize the Kullback–Leibler Divergence

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

Easy??

Estimated Reverse Process

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

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

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



Training of μ_θ and Σ_θ

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 μ_θ and Σ_θ

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

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

Training of μ_θ and Σ_θ

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 μ_θ and Σ_θ

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 μ_θ and Σ_θ

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 μ_θ and Σ_θ

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 μ_θ and Σ_θ

...after some algebraic steps :)

Reformulated Loss Function

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

where,

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

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

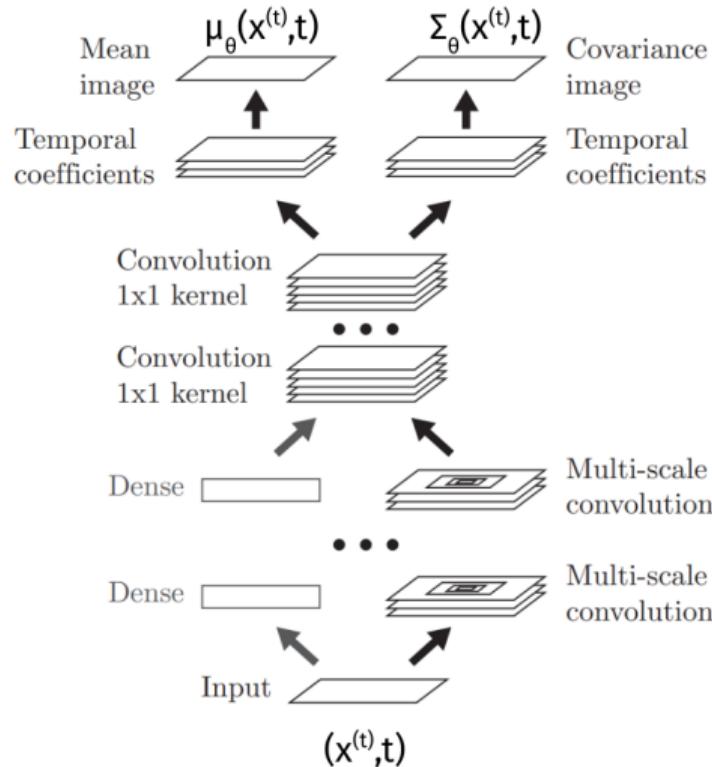
$$\mathcal{L}_0 = \mathbb{E}_{q(\mathbf{x}^{(0\dots T)})} \left[p_\theta(\mathbf{x}^{(0)} | \mathbf{x}^{(1)}) \right]$$

Note.

\mathcal{L}_T is constant.

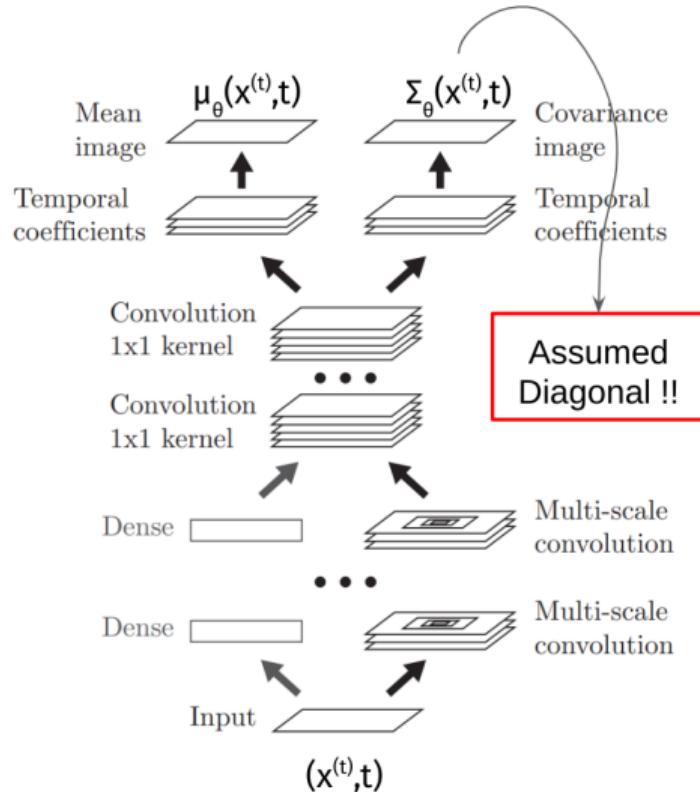
$\mathcal{L}_0, \mathcal{L}_t$ explicit.

Neural Network that estimate μ_θ and Σ_θ



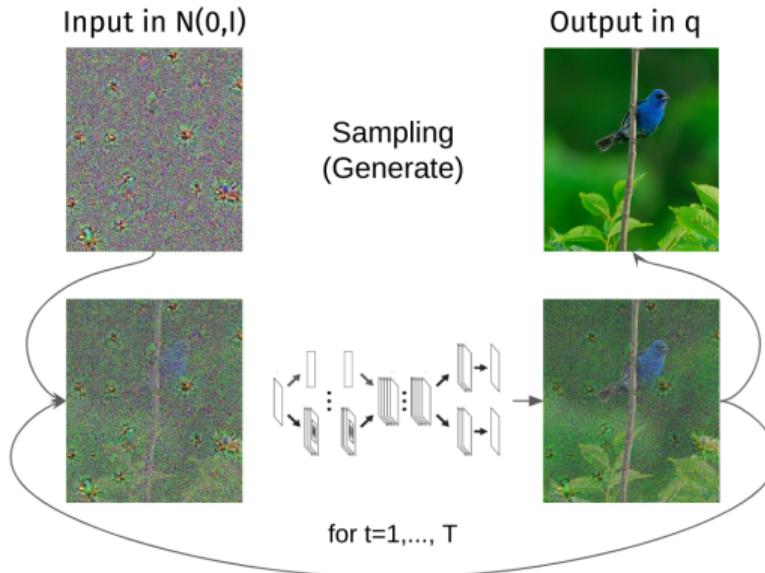
Proposed Neural Network for CIFAR10 image generation. T=1000

Neural Network that estimate μ_θ and Σ_θ



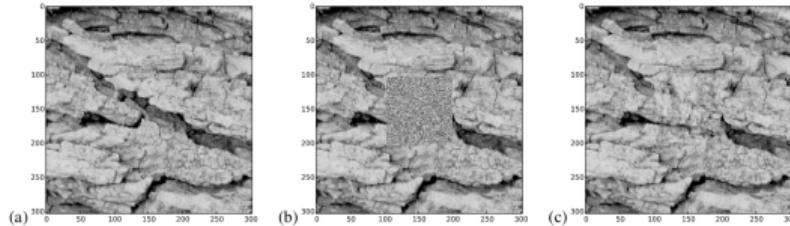
Proposed Neural Network for CIFAR10 image generation. T=1000

Sampling or Generative Stage



Experiments⁶

Bark Dataset



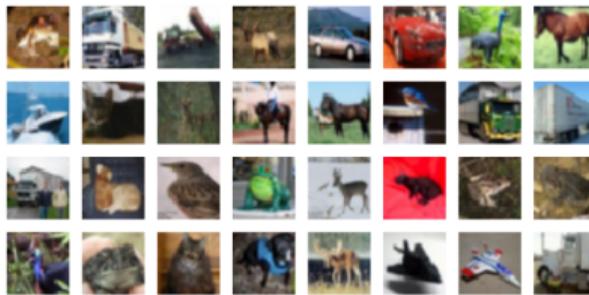
MNIST

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

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

Experiments⁷

CIFAR10 (original)



CIFAR10 (generated)



⁷Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

Timeline

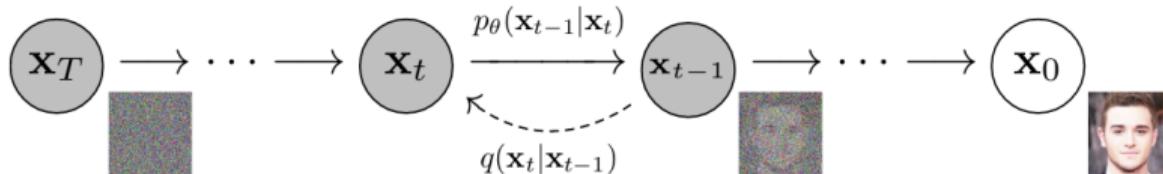
2015) ...*Non-equilibrium Thermodynamics*. Sohl-Dickstein et al. ICML. ✓

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...⁸



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

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

⁸Ho, 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

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

Denoising Diffusion Probabilistic Model

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

Simplification II: Estimating the committed error

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

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

Denoising Diffusion Probabilistic Model

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

Simplification II: Estimating the committed error

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

$\varepsilon_\theta(\mathbf{x}^{(t)}, t)$ 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

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

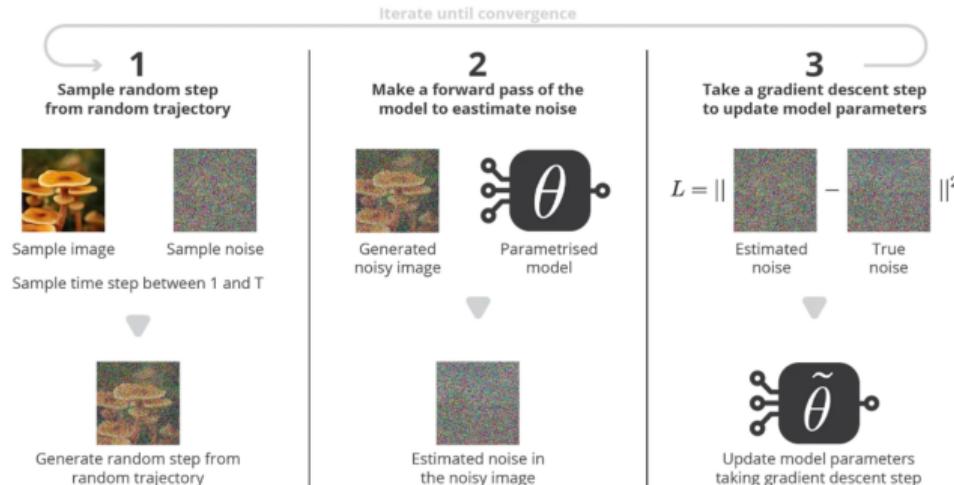
Training and Sampling Procedure

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

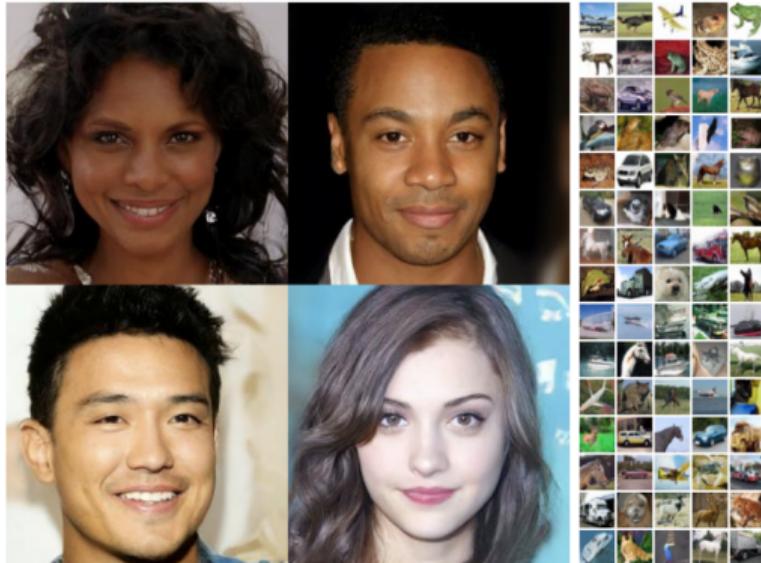


Figure 1: Generated samples on CelebA-HQ 256×256 (left) and unconditional CIFAR10 (right)

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

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”

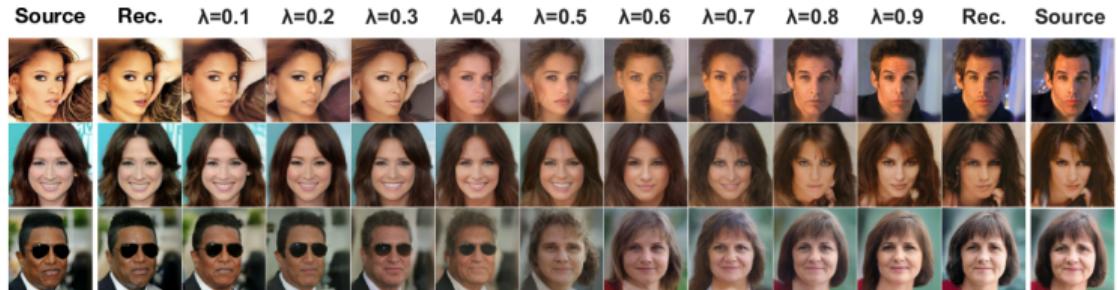
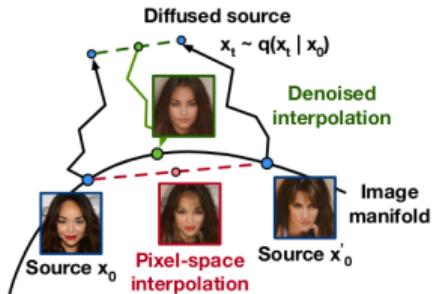
Table 1: CIFAR10 results. NLL measured in bits/dim.

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

CIFAR10 results. NLL measured in bits/dim¹⁰

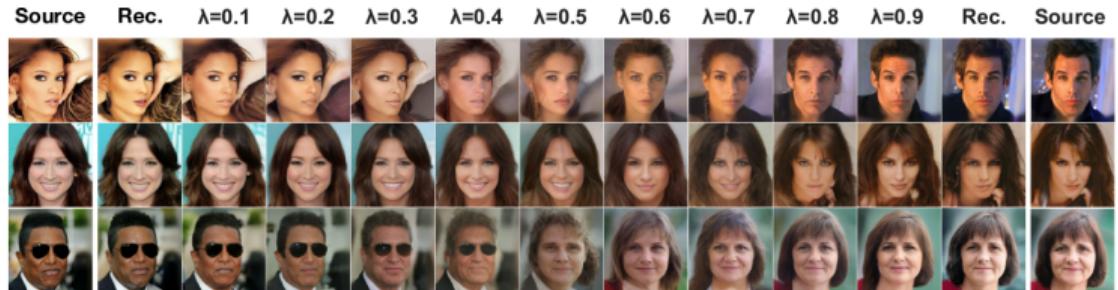
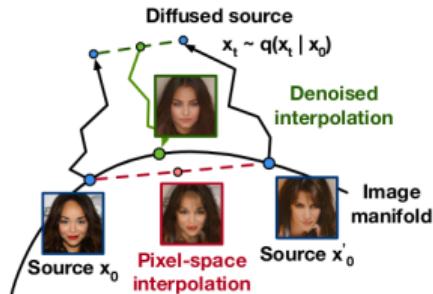
¹⁰Ho, Jain, and Abbeel, “Denoising Diffusion Probabilistic Models”.

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



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

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

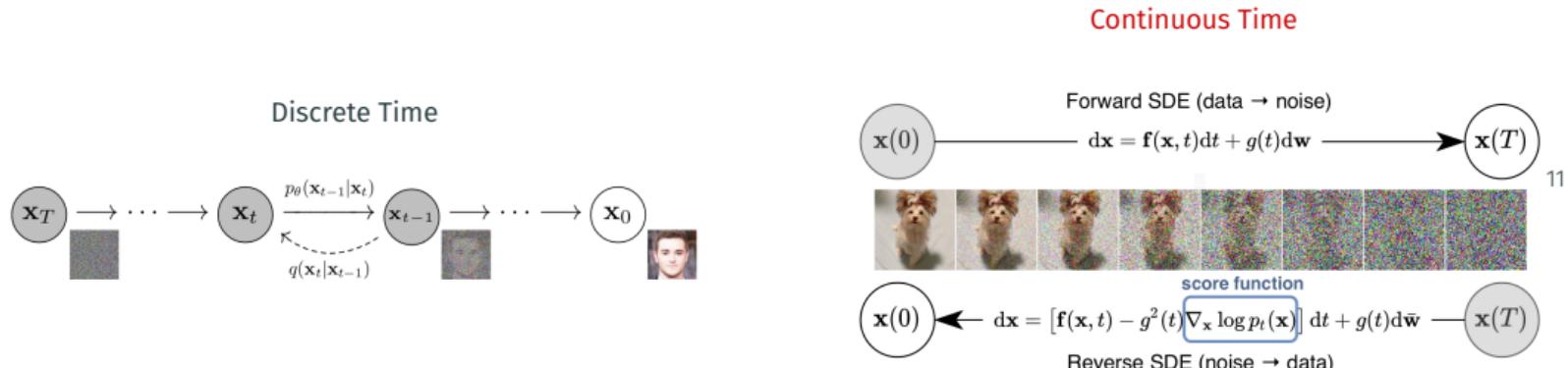
Timeline

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 $p_t(\mathbf{x})$;

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

Continuous Diffusion Process described by SDE

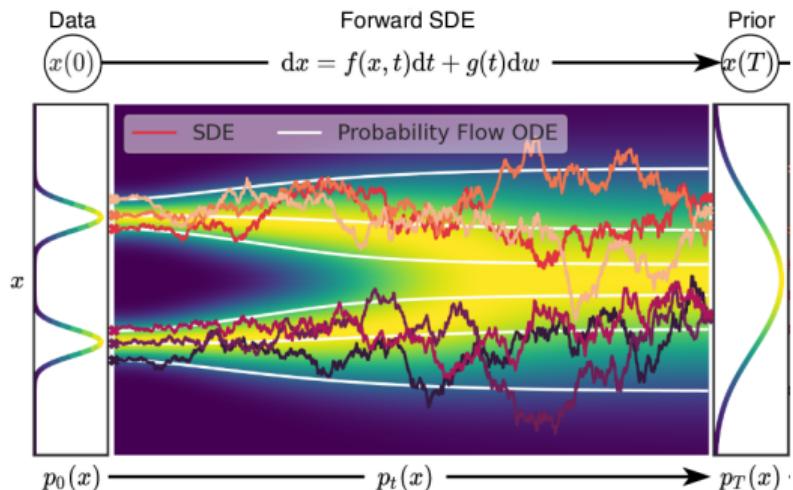
Continuous Diffusion Process

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

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 $\nabla_x p_t(\mathbf{x})$

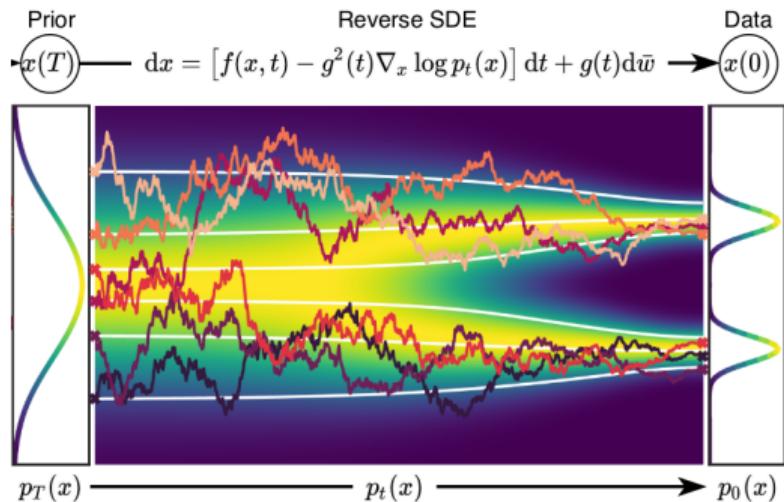
Theorem

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



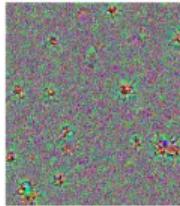
DALL-E2



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

¹²Credits: 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



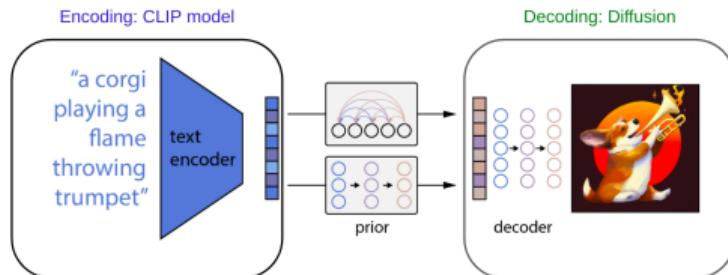
12

¹²Credits: DALL-E2 website

Overview: CLIP + Diffusion

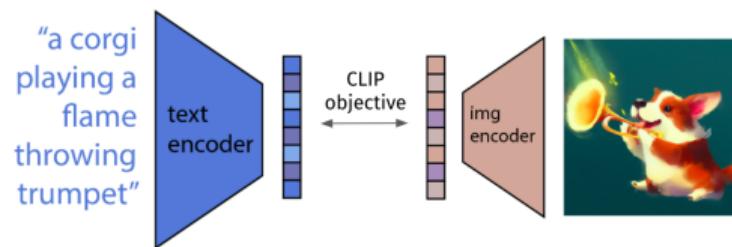
13

Text-to-Image Generation with CLIP



Diffusion models allows generating images with high sample fidelity and photorealism

CLIP model

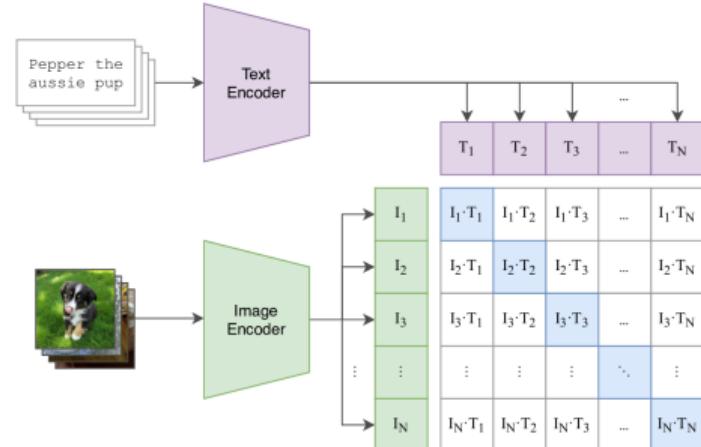


Embedding of images and text in the same latent space

¹³Ramesh 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.

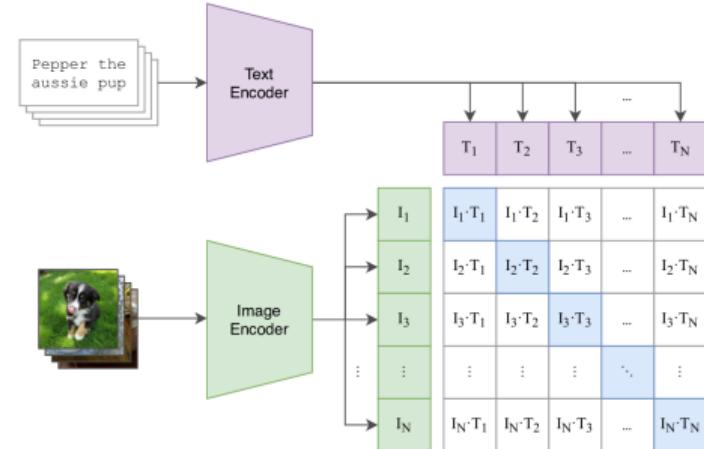


CLIP allows embedding of images and text in the same latent space.

¹⁴ Radford et al., "Learning Transferable Visual Models From Natural Language Supervision".

CLIP: Latent Embedding model

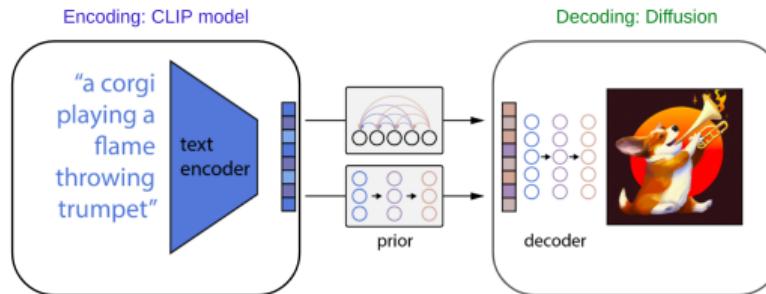
4. Aim: Zero-shot classification (of unseen datasets, see later.)
5. The Text Encoder is a Transformer for NLP (63M of parameters, next lectures).
6. The Image Encoder include ResNet-50 and Vision-Transformers



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

¹⁴ Radford et al., "Learning Transferable Visual Models From Natural Language Supervision".

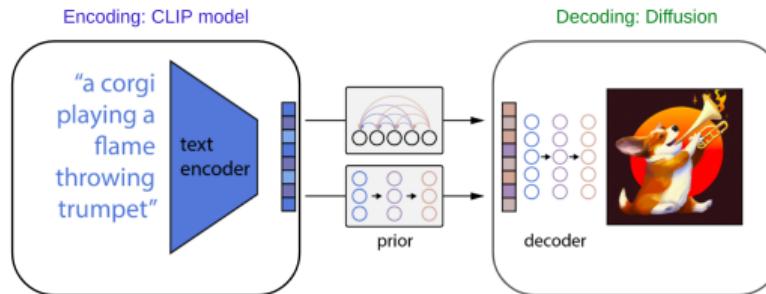
DALL-E2 with higher detail



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



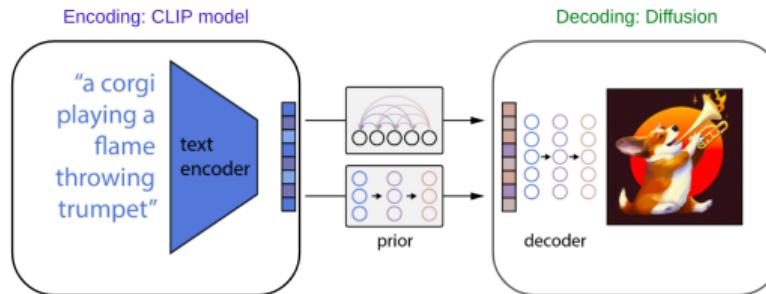
Let (x, y) be an (image, caption) pair.

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

Provide an image embedding conditioned to a text.

Provide an Image conditioned to a text and Image Emb.

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 $q(x | z_i, y)$

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

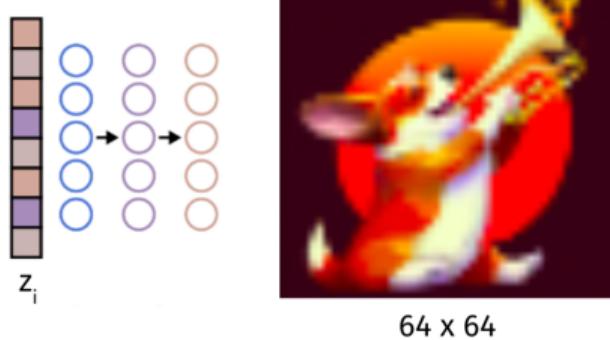
Observation

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

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.



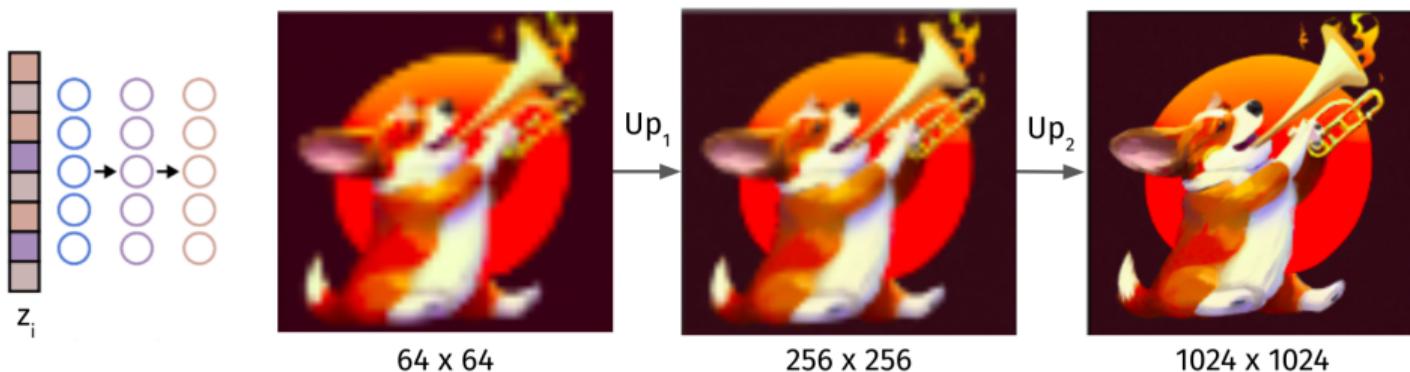
Decoding through Diffusion models

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.

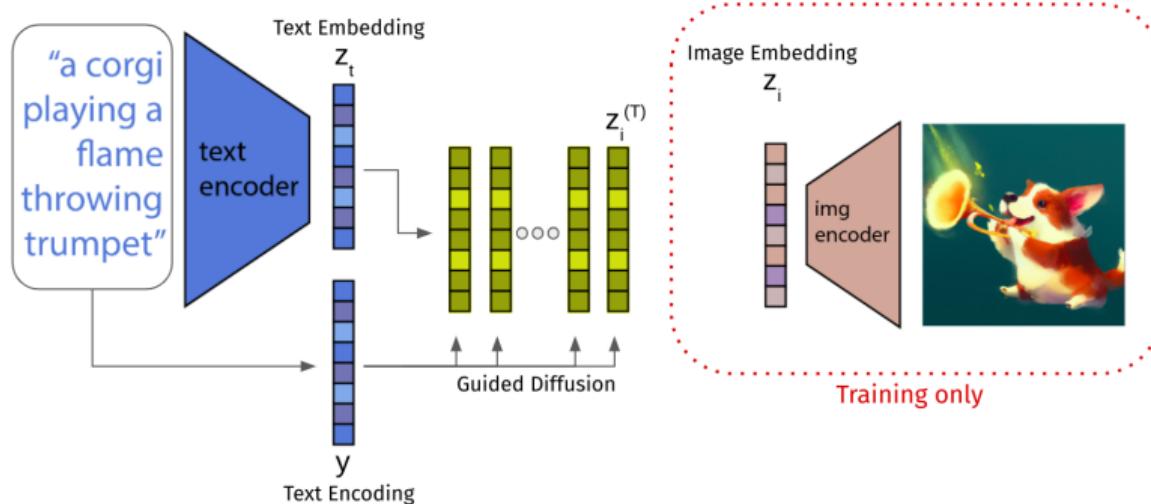
Step 2. Upsampling Procedure

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



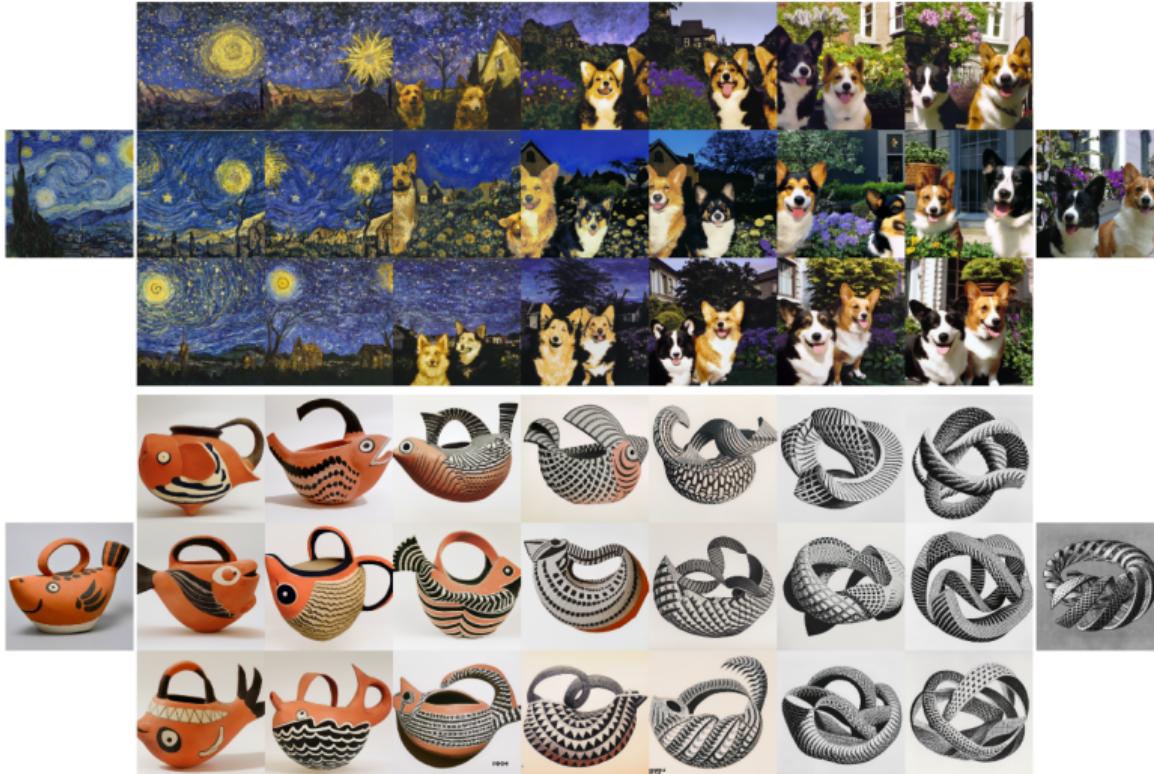
Prior

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



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

¹⁵Ho, Jain, and Abbeel, “Denoising Diffusion Probabilistic Models”.

1. Diffusion models, as generative models, can be used for malicious purpose. 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**.

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

¹⁵ 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

Fabio Brau

 Scuola Superiore Sant'Anna, Pisa

 fabio.brau@santannapisa.it

 retis.santannapisa.it/~f.brau

 linkedin.com/in/fabio-brau

TELECOMMUNICATIONS,
COMPUTER
ENGINEERING,
AND PHOTONICS
INSTITUTE



Sant'Anna
School of Advanced Studies – Pisa

ECCELLENZA
MIUR 2018-2022



Sant'Anna
Scuola Universitaria Superiore Pisa


Retis
Real-Time Systems Laboratory

Proof Details



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 $(1 - \beta_{t+1})\alpha_t + \beta_{t+1}$.

