Diffusion Models: DALL-E

Deep Learning and Neural Networks: Advanced Topics

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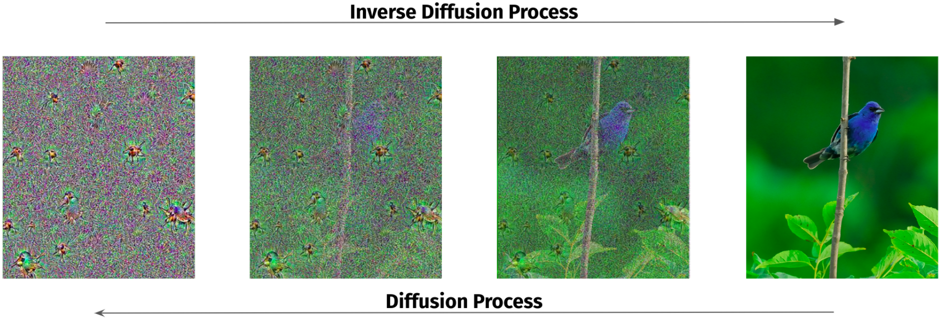
Introduction

Diffusion Models

Overview

Diffusion models are generative models that aim at denoising data



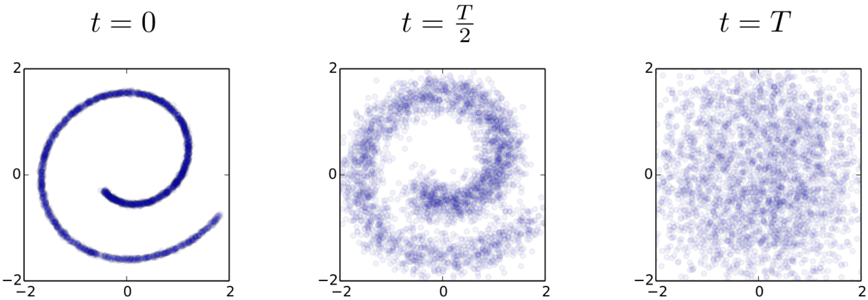
Timeline

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.

Deep Unsupervised Learning using Non-Equilibrium Thermodynamics



Diffusion process as a **Markov Chain** with **Continuous State Space** and **Discrete Time**.[1]

[1] Sohl-Dickstein et al., "Deep Unsupervised Learning using Nonequilibrium Thermodynamics".

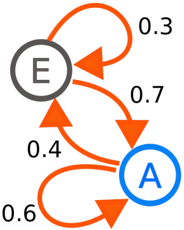
Reminder: Markov Chains with Discrete Time

Informal Definition

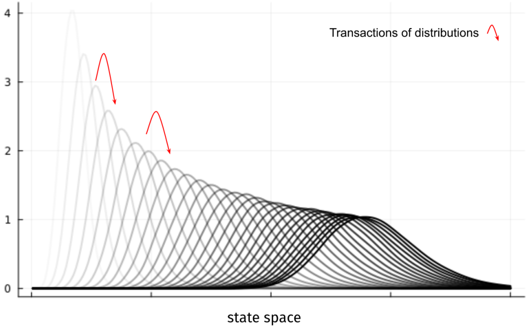
A sequence of random variables $\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(t)}, \cdots$, such that:

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

Discrete State Space S



Continuous State Space S



Reminder: MCDT with Discrete State Space

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

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

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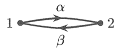
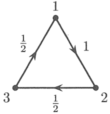
P is a stochastic matrix!

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

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



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



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

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

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

$$p\left(\mathbf{x}, \mathbf{y}\right) = p(\mathbf{x} \,|\, \mathbf{y}) \, p\left(\mathbf{y}\right)$$

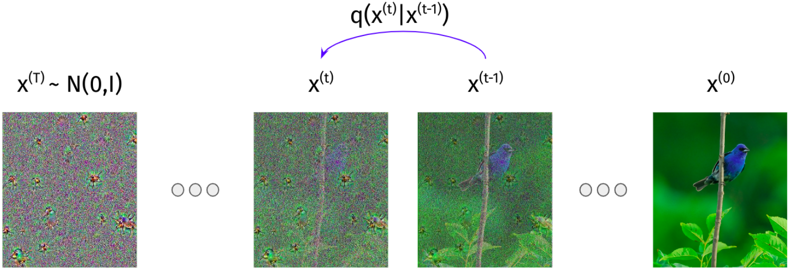
Marginal Distribution $p(\mathbf{x})$

$$p\left(\mathbf{x}\right) = \int_S p\left(\mathbf{x}, \mathbf{y}\right) \, d\mathbf{y} = \int_S p(\mathbf{x} \,|\, \mathbf{y}) \, p\left(\mathbf{y}\right) \, d\mathbf{y}$$

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: $\beta_1, \cdots, \beta_T \in (0, 1]$



Forward Diffusion Process

"Adding noise to data..."

- Data Distribution: $\mathbf{x}^{(0)} \sim q$ Not Analytic!!
- Transaction Kernel: $q\left(\mathbf{x}^{(t)} \mid \mathbf{x}^{(t-1)}\right) = \mathcal{N}\left(\mathbf{x}^{(t)}; \sqrt{1-\beta_t}\mathbf{x}^{(t-1)}; \beta_t I\right)$
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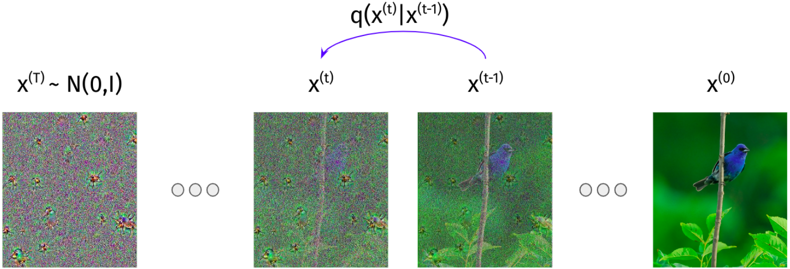

Forward Diffusion Process: Explicit Representation

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

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...

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

Forward Diffusion Process: Distribution Representation

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

Forward Diffusion Process: Distribution Representation

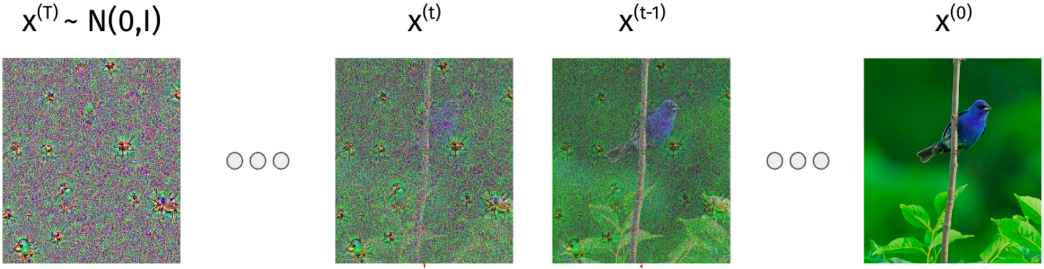
Markov property allows breaking up distributional Representation...

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

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



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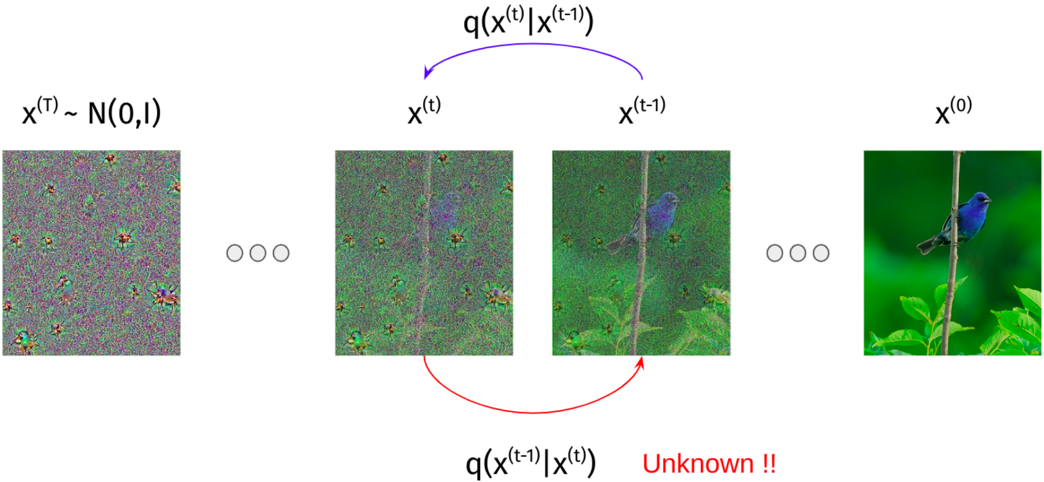

Reverse Diffusion Process

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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Theorem. Reverse of Gaussian DP is $\approx$ Gaussian DP[2]

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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Reverse Diffusion Process

Forward Diffusion Process

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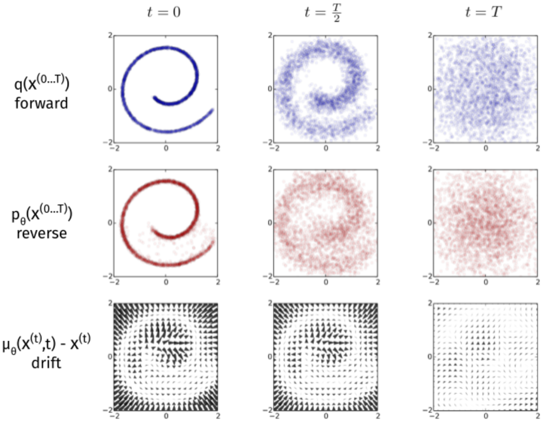
Mean $\boldsymbol{\mu}_\theta$ and covariance $\boldsymbol{\Sigma}_\theta$ have to be learned!!

[2] Sohl-Dickstein et al., “Deep Unsupervised Learning using Nonequilibrium Thermodynamics”.

Visualization of Diffusion Process: 2D dimensional case



[3]

[3] Sohl-Dickstein et al., “Deep Unsupervised Learning using Nonequilibrium Thermodynamics”.

Training of $\boldsymbol{\mu}_\theta$ and Σ_θ

Aim

Seach for the best parameters θ

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

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

Estimated Reverse Process

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

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

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Method

Minimize the *Kullback–Leibler* Divergence

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

Training of μ_θ and Σ_θ

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Easy??

Training of $\boldsymbol{\mu}_\theta$ and Σ_θ

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Easy??

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

Broader Impacts

CLIP Model

"We also found discrepancies across gender and race for people categorized into the 'crime' and 'non-human' categories..."[4]

[4] Radford et al., "Learning Transferable Visual Models From Natural Language Supervision".

Thanks for the attention

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