KSBi-BIML 2024

Bioinformatics & Machine Learning(BIML) Workshop for Life and Medical Scientists

생명정보학 & 머신러닝 워크샵 (온라인)

Diffusion Models – 이해와 응용

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KSBI KOREAN SOCIETY FOR BIOINFORMATICS | 한국생명정보학회

본 강의 자료는 한국생명정보학회가 주관하는 BIML 2024 워크샵 온라인 수업을 목적으로 제작된 것으로 해당 목적 이외의 다른 용도로 사용할 수 없음을 분명하게 알립니다.

이를 다른 사람과 공유하거나 복제, 배포, 전송할 수 없으며 만약 이러한 사항을 위반할 경우 발생하는 **모든 법적 책임은 전적으로 불법 행위자 본인에게 있음을 경고**합니다.

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안녕하십니까?

한국생명정보학회가 개최하는 동계 교육 워크샵인 BIML-2024에 여러분을 초대합니다. 생명정보학 분야의 연구자들에게 최신 동향의 데이터 분석기술을 이론과 실습을 겸비해 전달하고자 도입한 전문 교육 프로그램인 BIML 워크샵은 2015년에 시작하여 올해로 벌써 10년 차를 맞이하게 되었습니다. BIML 워크샵은 국내 생명정보학 분야의 최초이자 최고 수준의 교육프로그램으로 크게 인공지능과 생명정보분석 두 개의 분야로 구성되어 있습니다. 올해 인공지능 분야에서는 최근 생명정보 분석에서도 응용이 확대되고 있는 다양한 인공지능 기반 자료모델링 기법들에 대한 현장 강의가 진행될 예정이며, 관련하여 심층학습을 이용한 단백질구조예측, 유전체분석, 신약개발에 대한 이론과 실습 강의가 함께 제공될 예정입니다. 또한 단일세포오믹스, 공간오믹스, 메타오믹스, 그리고 롱리드염기서열 자료 분석에 대한 현장 강의는 많은 연구자의 연구 수월성 확보에 큰 도움을 줄 것으로 기대하고 있습니다.

올해 BIML의 가장 큰 변화는 최근 연구 수요가 급증하고 있는 의료정보자료 분석에 대한 현장 강의를 추가하였다는 것입니다. 특히 의료정보자료 분석을 많이 수행하시는 의과학자 및 의료정보 연구자들께서 본 강좌를 통해 많은 도움을 받으실 수 있기를 기대하고 있습니다. 또한 다양한 생명정보학 분야에 대한 온라인 강좌 프로그램도 점차 증가하고 있는 생명정보 분석기술의 다양화에 발맞추기 위해 작년과 비교해 5강좌 이상을 신규로 추가했습니다. 올해는 무료 강좌 5개를 포함하여 35개 이상의 온라인 강좌가 개설되어 제공되며, 연구 주제에 따른 연관된 강좌 추천 및 강연료 할인 프로그램도 제공되며, 온라인을 통한 Q&A 세션도 마련될 예정입니다. BIML-2024는 국내 주요 연구중심 대학의 전임 교원이자 각 분야 최고 전문가들의 강의로 구성되었기에 해당 분야의 기초부터 최신 연구 동향까지 포함하는 수준 높은 내용의 강의가 될 것이라 확신합니다.

BIML-2024을 준비하기까지 너무나 많은 수고를 해주신 운영위원회의 정성원, 우현구, 백대현, 김태민, 김준일, 김상우, 장혜식, 박종은 교수님과 KOBIC 이병욱 박사님께 커다란 감사를 드립니다. 마지막으로 부족한 시간에도 불구하고 강의 부탁을 흔쾌히 허락하시고 훌륭한 현장 강의와 온라인 강의를 준비하시는데 노고를 아끼지 않으신 모든 강사분들께 깊은 감사를 드립니다.

2024년 2월

한국생명정보학회장 이 인 석

강의개요

Diffusion Models - 이해와 응용

최근의 생성모델의 성능 향상은 새로운 형태의 인공지능 응용 가능성을 보여주고 있다. 본 강의에서는 생성모델 가운데 하나인 Diffusion 모델을 설명한다. 가우시안을 통한 추론 방법의 이해에서 시작하여 Diffusion 모델의 수식을 이해하고, diffusion 모델이 다른 생성 모델과 근본적으로 어떻게 다른지에 대한 논의를 제공할 예정이다. 간단한 실습을 통해 diffusion 모델이 어떻게 작동하는지 살펴본다.

- Diffusion model 개요 및 다른 생성모델과의 개념 비교
- Diffusion 작용과 역작용을 위한 노이즈 예측
- 데이터 생성의 간단한 실습

* 참고논문:

1. Jonathan Ho, Ajay Jain, Pieter Abbeel (2020) Denoising diffusion probabilistic models, *Advances in Neural Information Processing Systems 33*
2. Jonathan Ho, Tim Salimans (2022) Classifier-Free Diffusion Guidance, *arXiv:2207.12598*

* 교육생준비물:

노트북 (웹브라우저로 구글 CoLab을 실행시킬 수 있는 노트북)

* 강의 난이도: 중급

* 강의: 노영균 교수 (한양대학교 컴퓨터소프트웨어학부 / 고등과학원 계산과학부)

Curriculum Vitae

Speaker Name: Yung-Kyun Noh, Ph.D.

▶ **Personal Info**

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Affiliation	1. Department of Artificial Intelligence, Hanyang University 2. Department of Computer Science, Hanyang University 3. School of Computational Sciences, Korea Institute for Advanced Study

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Research Interest

Machine Learning, Nonparametric methods, Information theory

Educational Experience

1998	B.S. in Physics, POSTECH, Rep. of Korea
2011	Ph.D. in Computer Science (Interdisciplinary Program in Cognitive Science), Seoul National University, Rep. of Korea

Professional Experience

2007-2012	Visiting Scholar, Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, PA, U.S.A.
2019-2021	Assistant Professor, Department of Computer Science, Hanyang University, Seoul, Korea
2019-2021	Associate Member, School of Computational Sciences, Korea Institute for Advanced Study, Seoul, Korea
2020-2021	Visiting Scientist, Gastroenterology and Hepatology, Mayo Clinic, Rochester, MN, USA
2018-	Visiting Scientist, RIKEN Center for Advanced Intelligence Project (AIP), Tokyo, Japan
2021-	Affiliate Professor, School of Computational Sciences, Korea Institute for Advanced Study, Seoul, Korea
2021-	Associate Professor, Department of Computer Science, Hanyang University, Seoul, Korea
2022-	Research Collaborator, Gastroenterology and Hepatology, Mayo Clinic, Rochester, MN, USA
2023-	Chair, Dept. of Artificial Intelligence, Hanyang University, Korea

Selected Publications (5 maximum)

1. Lee, J.-W., Won, J.-H., Jeon, S., Choo, Y., Yeon, Y., Oh, J.-S., Kim, M., Kim, S., Joung, I., Jang, C., Lee, S. J., Kim, T. H., Jin, K. H., Song, G., Kim, E.-S., Yoo, J., Paek, E., Noh, Y.-K., Joo, K. (2023) DeepFold: Enhancing Protein Structure Prediction Through Optimized Loss Functions, Improved Template Features, and Re-optimized Energy Function, *Bioinformatics, 39:12, btad712*
2. Yoon, S., Park, F. C., Yun, G. Kim, S., I., Noh, Y.-K. (2023) Variational Weighting for Kernel Density Ratios, *Advances in Neural Information Processing Systems 36 (NeurIPS)*
3. Yoon, S., Jin, Y.-U., Noh, Y.-K., Park, F. C. (2023) Energy-Based Models for Anomaly Detection: A Manifold Diffusion Recovery Approach, *Advances in Neural Information Processing Systems 36 (NeurIPS)*
4. Jang, C., Lee, S., F. C. Park, Y.-K. Noh (2022) A Reparametrization-Invariant Sharpness Measure Based on Information Geometry, *Advances in Neural Information Processing Systems 35 (NeurIPS)*
5. Lee, H., Lee, J., Choi, Y., Jeon, W., Lee, B.-J., Noh, Y.-K., Kim, K.-E. (2022) Local Metric Learning for Off-Policy Evaluation in Contextual Bandits with Continuous Actions, *Advances in Neural Information Processing Systems 35 (NeurIPS)*

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Diffusion Models - 이해와 응용

노영균 (한양대학교 & 고등과학원)

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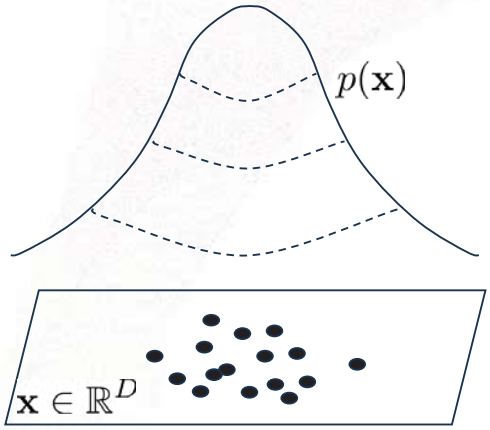
Data generation

$\mathbf{x} \sim p(\mathbf{x})$



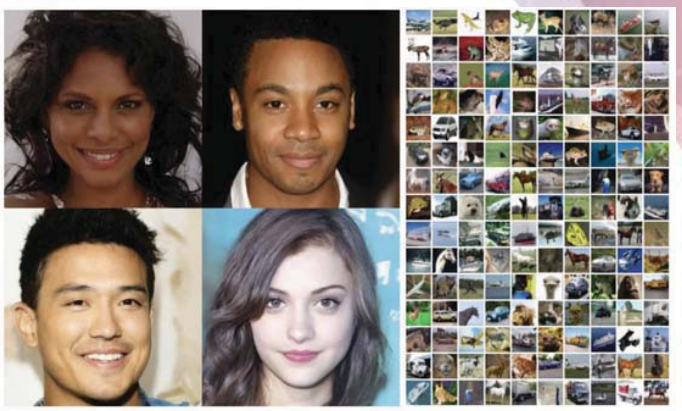


Figure 1: Generated samples on CelebA-HQ 256 × 256 (left) and unconditional CIFAR10 (right)

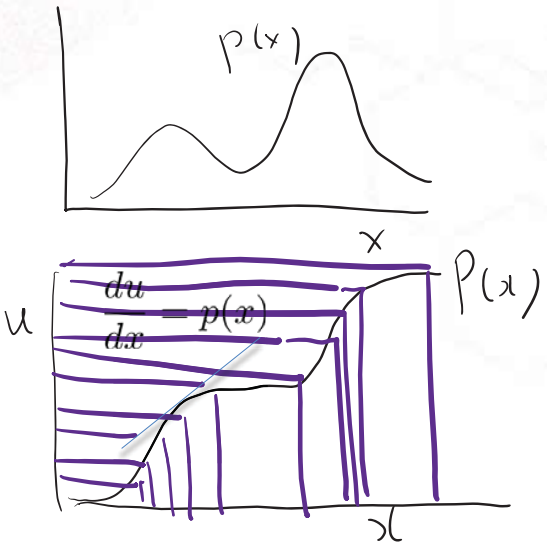
$\mathbf{x} \in \mathbb{R}^{\text{Pixel}}$

Data generation 101

Cumulative distribution

$$P(x) = \int_{-\infty}^{x} p(x)dx \equiv u$$

$$x = P^{-1}(u)$$



$$du = p(x)dx$$

$$u \sim \mathrm{Unif}(0, 1)$$

$$\int_{-\infty}^{u} p(u)du = \int_{0}^{u} du = \int_{-\infty}^{P^{-1}(u)} p(x)dx, \quad 0 \le u \le 1$$

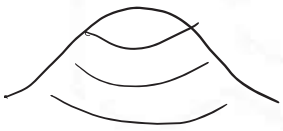
Flow-based model (Normalizing flow)

$p(\mathbf{x})d\mathbf{x} = p(\mathbf{u})d\mathbf{u}$, $\mathbf{x} = T(\mathbf{u})$ (full-rank transformation)

$$p(\mathbf{x}) = p(\mathbf{u}) \left| \frac{d\mathbf{u}}{d\mathbf{x}} \right|$$

$$= p(\mathbf{u}) \det J_T^{-1}(\mathbf{u})$$

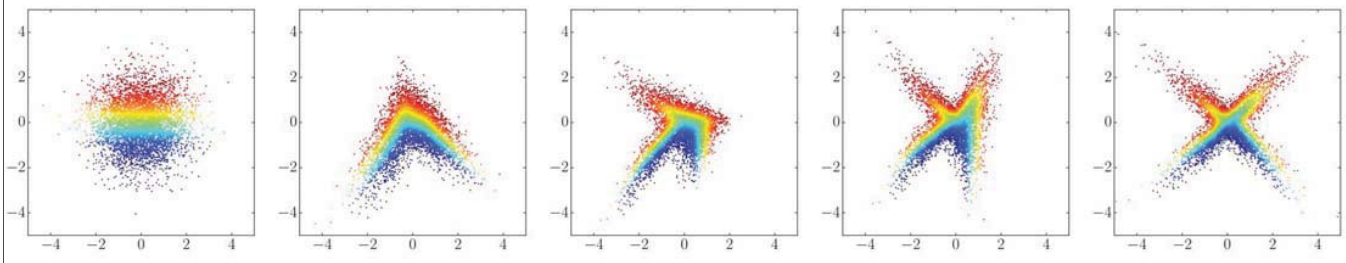
Base distribution $p_{\mathbf{u}}(\mathbf{u})$



Flow – Gradually transformed by the sequence of consecutive transformations $T_1, \ldots, T_K$

$$T = T_K \cdot T_{K-1} \cdots T_1$$

Normalizing – the inverse flow $T_K^{-1}, \ldots, T_1^1$



G. Papamakarios et al. JMLR 2021

Flow-based model (Normalizing flow)

Learning

Data $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^{N} \sim p(\mathbf{x})$

Prevent compression from x to u

$$\det J_T(\mathbf{u}_i) = \left|\frac{d\mathbf{x}}{d\mathbf{u}}\right|_{\mathbf{u}}$$

Maximum Likelihood

Minimize

Gaussian

$$L = \sum_{i=1}^{N} -\log p(\mathbf{x}_i) = \sum_{i=1}^{N} -\log p_{\mathbf{u}}(\mathbf{u}_i) - \log\det J_{T^{-1}}(\mathbf{u}_i)$$

$$\mathbf{u}_i = T^{-1}(\mathbf{x}_i)$$

Likelihood representation with respect to $p(\mathbf{u})$

The loss is sensitive to the volume change of transformation due to the determinant of Jacobian.

5

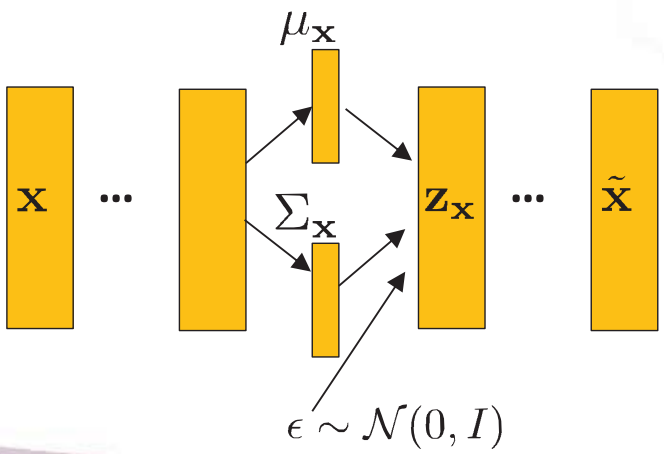
Deterministic flow:

Reversed flow is “exactly” the backward flow

Variational Autoencoder

$$L(\mathbf{x}) = \log p(\mathbf{x}|\mathbf{z}_\mathbf{x}) - KL(q_\mathbf{x}(\mathbf{z})||p(\mathbf{z}))$$
$$= -||\mathbf{x} - \tilde{\mathbf{x}}(\mathbf{z}_\mathbf{x})||^2 - KL(\mathcal{N}(\mu_\mathbf{x}, \Sigma_\mathbf{x})||\mathcal{N}(0, I))$$

Neural Networks (Decoder) *Neural Networks (Encoder)*



Variational Autoencoder

$p(\mathbf{x})$ $p(\mathbf{z}|\mathbf{x})$ ← Some appropriate mapping

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

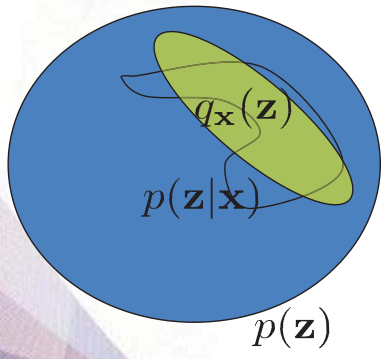
$p(\mathbf{x}|\mathbf{z})$

$$= \frac{p(\mathbf{x})p(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})}$$

$q_\mathbf{x}(\mathbf{z})$: Gaussian

$$= \mathcal{N}(\mu_\mathbf{x}, \Sigma_\mathbf{x})$$

$$\mathbf{z} \in \mathbb{R}^{D_\mathbf{z}} \rightarrow$$
$$\mu_\mathbf{x} \in \mathbb{R}^{D_\mathbf{z}}, \Sigma_\mathbf{x} \in \mathbb{R}^{D_\mathbf{z} \times D_\mathbf{z}}$$



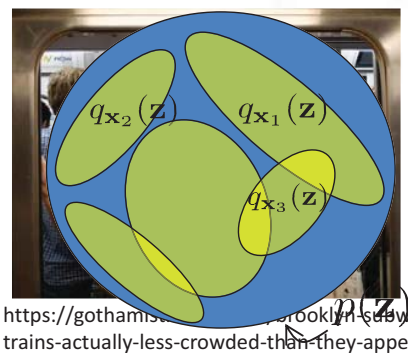
Reparametrization from $q_\mathbf{x}(\mathbf{z})$

Optimize

$||\mathbf{x} - f(\mathbf{z})||^2 \downarrow$

$KL(q_\mathbf{x}, p(\mathbf{z})) \downarrow$

Then

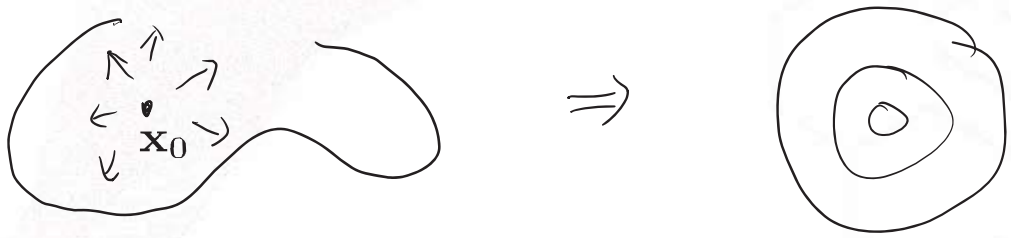


https://gothamist.com/.../brooklyn-subway-trains-actually-less-crowded-than-they-appear

Diffusion models

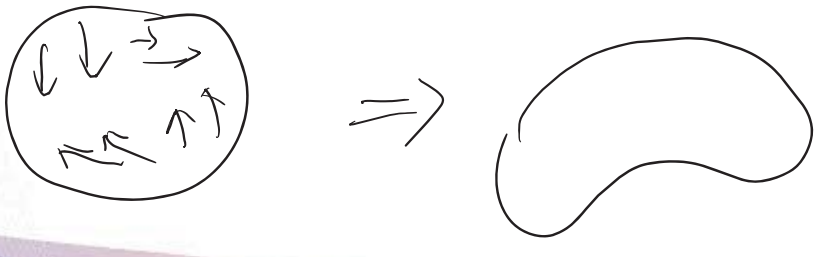
- Forward process

  Pick up $\mathbf{x}_0 \sim p(\mathbf{x})$, then randomly move



- Reverse process

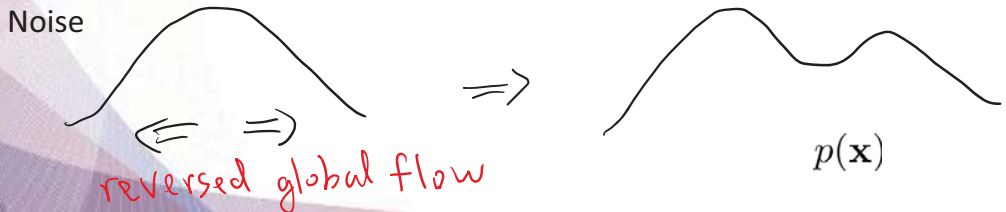
  How does backward process make flow?



Diffusion models

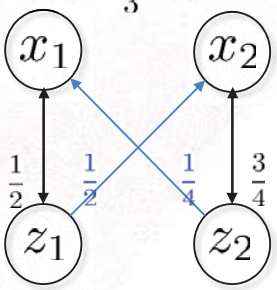
Diffusion of Non-uniform density makes a global flow

Reverse process in diffusion model reconstructs the backward global flow.



Forward-Reverse process

$$p(x = x_1) = \frac{1}{3} \quad p(x = x_2) = \frac{2}{3}$$



$$p(z = z_1) = \frac{1}{3} \quad p(z = z_2) = \frac{2}{3}$$

Forward process

$$p(z_1|x_1) = 1$$

$$p(z_2|x_2) = 1$$

Reverse process

$$p(x_1|z_1) = 1$$

$$p(x_2|z_2) = 1$$

Any process that preserves marginal will work. Do not consider joint density over x and z.

Reverse process

$$p(x_1|z_1) = \frac{1}{2} \quad p(x_2|z_1) = \frac{1}{2}$$

$$p(x_2|z_2) = \frac{3}{4} \quad p(x_2|z_2) = \frac{1}{4}$$

$$\vdots$$

Underlying diffusion procedure

Data

$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}) \qquad \mathbf{x}_0 \sim q(\mathbf{x}_0)$$

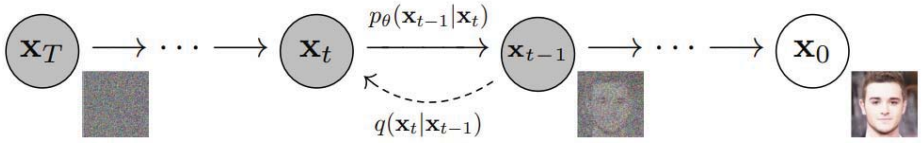


Figure 2: The directed graphical model considered in this work.

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) := \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}), \qquad q(\mathbf{x}_t|\mathbf{x}_{t-1}) := \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

$$\beta_t > 0$$

$q(\mathbf{x}_{1:T}|\mathbf{x}_0)$, $q(\mathbf{x}_t|\mathbf{x}_{t-1})$: Gaussians

Caution) $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$: Not Gaussian

If $p(\mathbf{x}_0)$ is Gaussian, $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is Gaussian.

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) = \int q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)p(\mathbf{x}_0)d\mathbf{x}_0$$

: Gaussian mixture

Model for reverse process

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

Objective function:

$$\mathbb{E}\left[-\log p_\theta(\mathbf{x}_0)\right] \leq \mathbb{E}_q\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right]$$

$$= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] =: L$$

Look at the derivations in the next two pages…

Objective function - 1

$$L = \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right]$$

$$= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t)} \cdot \frac{q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)}\right]$$

$$= \mathbb{E}_q\left[-\log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T)} - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t)} - \log q(\mathbf{x}_0)\right]$$

$$= D_{\mathrm{KL}}(q(\mathbf{x}_T) \parallel p(\mathbf{x}_T)) + \mathbb{E}_q\left[\sum_{t\geq 1} D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))\right] + H(\mathbf{x}_0)$$

Can we have this density function?

Objective function - 2

$$
\begin{aligned}
L &= \mathbb{E}_q\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] \\
&= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1}\log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] \\
&= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t>1}\log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} - \log \frac{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_1|\mathbf{x}_0)}\right] \\
&= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t>1}\log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)}\cdot\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} - \log \frac{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_1|\mathbf{x}_0)}\right] \\
&= \mathbb{E}_q\left[-\log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} - \sum_{t>1}\log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)} - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)\right] \\
&= \mathbb{E}_q\Bigg[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)\parallel p(\mathbf{x}_T))}_{L_T} + \underbrace{\sum_{t>1} D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)\parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\Bigg] \qquad (22)
\end{aligned}
$$

Gaussians ∵ x_0 given

Tractable functions

$q(\mathbf{x}_{t-1}|\mathbf{x}_0)$

$q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)$

$q(\mathbf{x}_t|\mathbf{x}_0)$

} Gaussians

Decomposition for Gaussian inference

$$p(\mathbf{x}_a, \mathbf{x}_b)$$

$$= \frac{1}{\sqrt{2\pi}^D \left| \begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b \end{pmatrix} \right|^{\frac{1}{2}}} \exp\left(-\frac{1}{2} \begin{pmatrix} \mathbf{x}_a - \mu_a \\ \mathbf{x}_b - \mu_b \end{pmatrix}^\top \begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{x}_a - \mu_a \\ \mathbf{x}_b - \mu_b \end{pmatrix} \right)$$

$$\mu_{a|b} = \Sigma_{ab}\Sigma_b^{-1}(\mathbf{x}_b - \mu_b)$$

$$= C \exp\left(-\frac{1}{2} \left(\mathbf{x}_a - \Sigma_{ab}\Sigma_b^{-1}(\mathbf{x}_b - \mu_b)\right)^\top \left(\Sigma_a - \Sigma_{ab}\Sigma_b^{-1}\Sigma_{ba}\right)^{-1} \left(\mathbf{x}_a - \Sigma_{ab}\Sigma_b^{-1}(\mathbf{x}_b - \mu_b)\right) \right.$$

$$\left. -\frac{1}{2} (\mathbf{x}_b - \mu_b)^\top \Sigma_b^{-1} (\mathbf{x}_b - \mu_b) \right) \qquad \Sigma_{a|b} = \Sigma_a - \Sigma_{ab}\Sigma_b^{-1}\Sigma_{ba}$$

$$= C \exp\left(-\frac{1}{2} (\mathbf{x}_a - \mu_{a|b})^\top \Sigma_{a|b}^{-1} (\mathbf{x}_a - \mu_{a|b}) \right. \qquad = p(\mathbf{x}_a|\mathbf{x}_b)\ p(\mathbf{x}_b)$$

$$\left. -\frac{1}{2} (\mathbf{x}_b - \mu_b)^\top \Sigma_b^{-1} (\mathbf{x}_b - \mu_b) \right)$$

Decomposition for Gaussian inference

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \quad \begin{matrix} \mathbf{x}_a \in \mathbb{R}^{D_a} \\ \mathbf{x}_b \in \mathbb{R}^{D_b} \end{matrix} \qquad \mu = \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b \end{pmatrix}$$

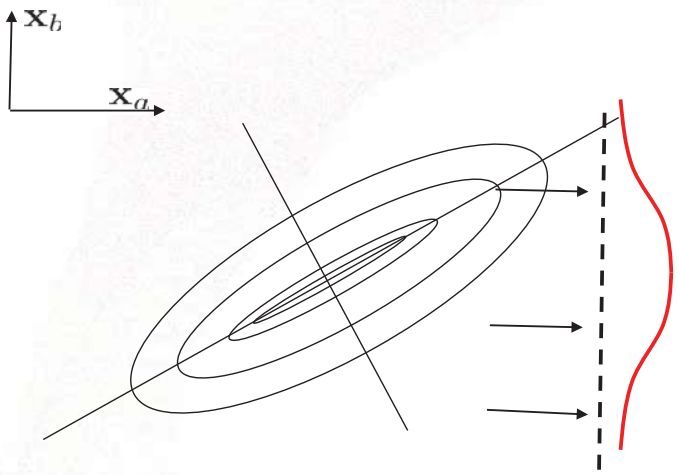
$$p(\mathbf{x}) = \frac{1}{\sqrt{2\pi}^D |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2} (\mathbf{x} - \mu)^\top \Sigma^{-1} (\mathbf{x} - \mu) \right)$$

$$= C_1 \exp\left(-\frac{1}{2} (\mathbf{x}_a - \mu_{a|b}(\mathbf{x}_b))^\top \Sigma_{a|b}^{-1} (\mathbf{x}_a - \mu_{a|b}(\mathbf{x}_b)) \right) \cdot$$

$$C_2 \exp\left(-\frac{1}{2} (\mathbf{x}_b - \mu_b)^\top \Sigma_b^{-1} (\mathbf{x}_b - \mu_b) \right)$$

$$p(\mathbf{x}) = p(\mathbf{x}_a, \mathbf{x}_b) = p(\mathbf{x}_a|\mathbf{x}_b) p(\mathbf{x}_b)$$

Gaussian random variable - marginalization



$$p(\mathbf{x}_b) = \int p(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_a$$
$$= \int p(\mathbf{x}_a|\mathbf{x}_b) p(\mathbf{x}_b) d\mathbf{x}_a$$
$$= \mathcal{N}(\mu_b, \Sigma_b)$$

Gaussian random variable - marginalization

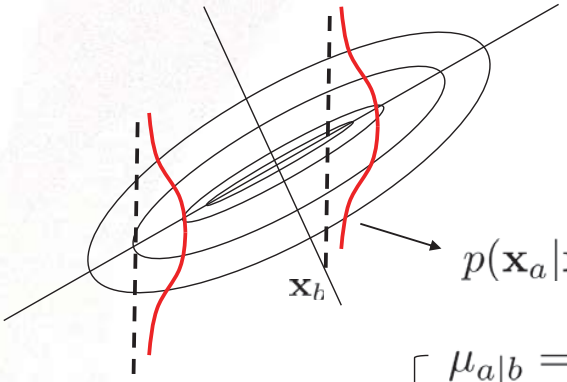
$$p(\mathbf{x}) = \frac{1}{\sqrt{2\pi}^D |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^\top \Sigma^{-1}(\mathbf{x}-\mu)\right)$$

$$p(\mathbf{x}_a, \mathbf{x}_b) = \frac{1}{\sqrt{2\pi}^D \left|\begin{pmatrix}\Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b\end{pmatrix}\right|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}\begin{pmatrix}\mathbf{x}_a-\mu_a \\ \mathbf{x}_b-\mu_b\end{pmatrix}^\top \begin{pmatrix}\Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b\end{pmatrix}^{-1} \begin{pmatrix}\mathbf{x}_a-\mu_a \\ \mathbf{x}_b-\mu_b\end{pmatrix}\right)$$

$$\int p(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_b = \frac{1}{\sqrt{2\pi}^{D_a} |\Sigma_a|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x}_a-\mu_a)^\top \Sigma_a^{-1}(\mathbf{x}_a-\mu_a)\right)$$
$$= \mathcal{N}(\mu_a, \Sigma_a)$$

Gaussian random variable - conditioning

$$p(\mathbf{x}) = \frac{1}{\sqrt{2\pi}^D |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^\top \Sigma^{-1}(\mathbf{x}-\mu)\right)$$



$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \quad \begin{matrix} \mathbf{x}_a \in \mathbb{R}^{D_a} \\ \mathbf{x}_b \in \mathbb{R}^{D_b} \end{matrix}$$

$$p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mu_{a|b}, \Sigma_{a|b})$$

$$\begin{cases} \mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_b^{-1}(\mathbf{x}_b - \mu_b) \\ \Sigma_{a|b} = \Sigma_a - \Sigma_{ab}\Sigma_b^{-1}\Sigma_{ba} \end{cases}$$

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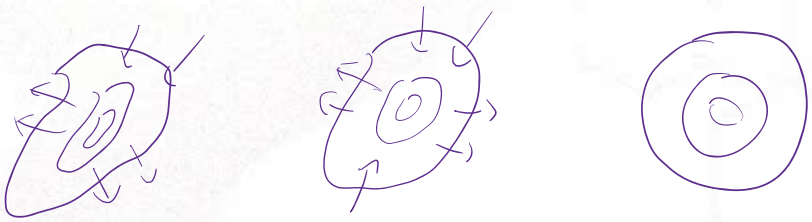
Diffusion and reverse process



$$x_t = \sqrt{1-\beta_t}\, x_{t-1} + \sqrt{\beta_t}\, \varepsilon_t \qquad \varepsilon_t \sim \mathcal{N}(0, I)$$

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$$L =$$

$$\mathbb{E}_q \Big[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0} \Big]$$

Given $\mathbf{x}_0$, everything is Gaussian. (Joint is not.)

$$\alpha_t := 1 - \beta_t \qquad \bar{\alpha}_t := \prod_{s=1}^{t} \alpha_s$$

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

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

$$\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}\mathbf{x}_t \quad \text{and} \quad \tilde{\beta}_t := \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t}\beta_t$$

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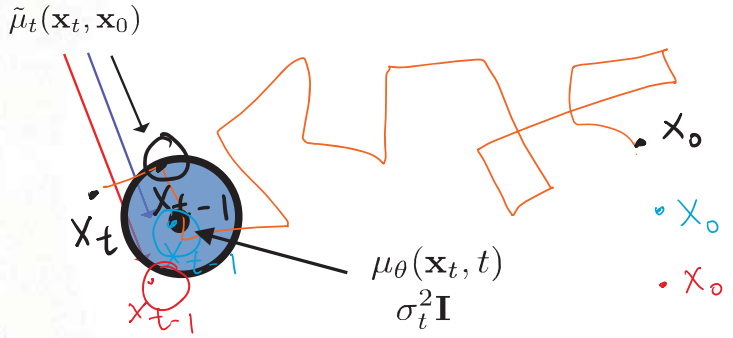
Learning

- Model

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \qquad \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t) = \sigma_t^2 \mathbf{I}$$

- K-L divergence:

$$L_{t-1} = \mathbb{E}_q \left[\frac{1}{2\sigma_t^2} \|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\|^2 \right] + C$$



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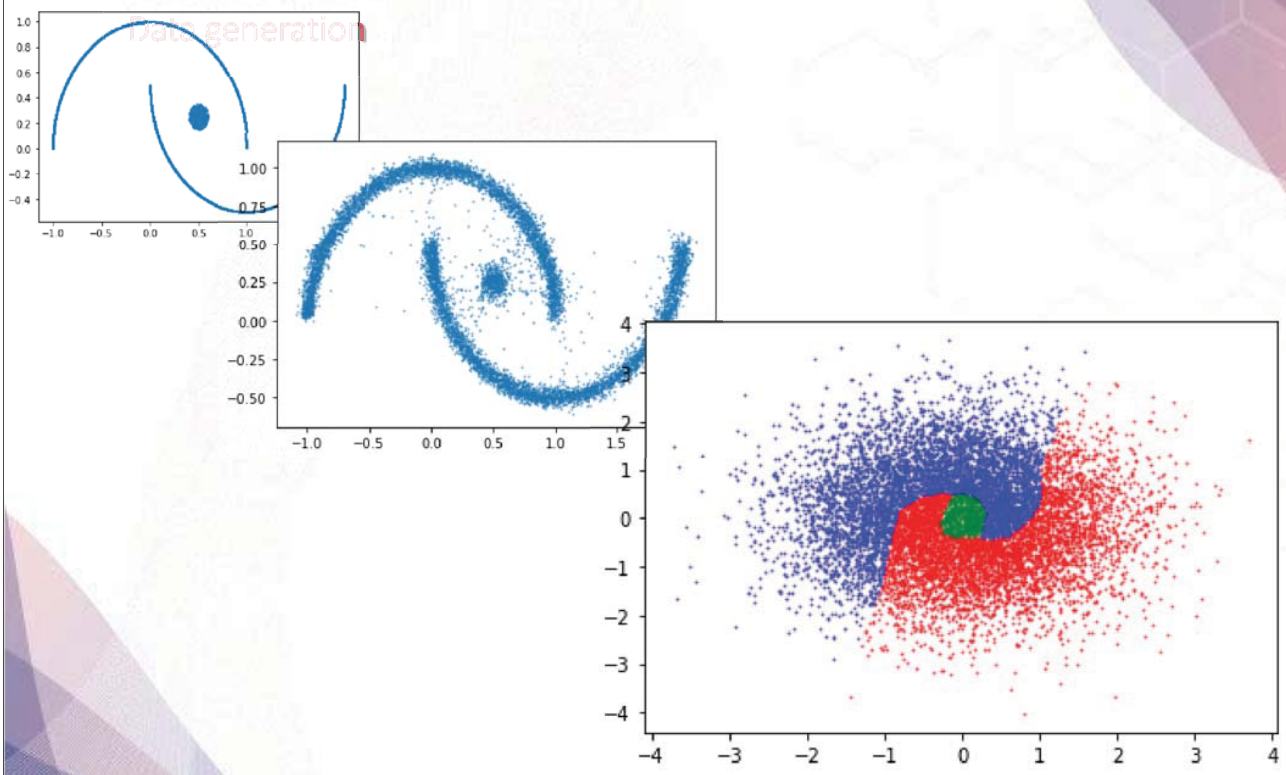

Conditional mean

$$\mathbf{x}_t(\mathbf{x}_0, \boldsymbol{\epsilon}) = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon} \qquad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$L_{t-1} - C \quad = \mathbf{x}_0$$

$$= \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{1}{2\sigma_t^2}\left\|\tilde{\boldsymbol{\mu}}_t\left(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon}), \frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon}) - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon})\right) - \boldsymbol{\mu}_\theta(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon}), t)\right\|^2\right]$$

$$= \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{1}{2\sigma_t^2}\left\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon}) - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right) - \boldsymbol{\mu}_\theta(\mathbf{x}_t(\mathbf{x}_0,\boldsymbol{\epsilon}), t)\right\|^2\right]$$

Recall

$$\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t \quad \text{and} \quad \tilde{\beta}_t := \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$$

$\boldsymbol{\mu}_\theta$ must predict $\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right)$ given $\mathbf{x}_t$

- Reparameterization

$$\boldsymbol{\mu}_\theta(\mathbf{x}_t, t) = \tilde{\boldsymbol{\mu}}_t\left(\mathbf{x}_t, \frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t))\right)$$

$$= \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)$$

$\boldsymbol{\epsilon}_\theta$ is a function approximator intended to predict $\boldsymbol{\epsilon}$ from $\mathbf{x}_t$

$$\mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2\right]$$

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Procedure

$$\mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2\right]$$

- From $\mathbf{x}_0$, generate $\mathbf{x}_t$, then predict ϵ.
- The distribution of $\epsilon_\theta(\mathbf{x}_t, \mathbf{x}_0)$ is determined by the distribution of $\mathbf{x}_0$. "Distribution of ϵ is isotropic Gaussian (non-informative)."
- Given $\mathbf{x}_0$, the distribution of ε should be non-informative. After marginalization, the expectation is the global flow of data due to diffusion.

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Algorithm 1 Training

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

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

Adding noise

Figure 6: Unconditional CIFAR10 progressive generation ($\hat{\mathbf{x}}_0$ over time, from left to right). Extended samples and sample quality metrics over time in the appendix (Figs. 10 and 14).

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Results

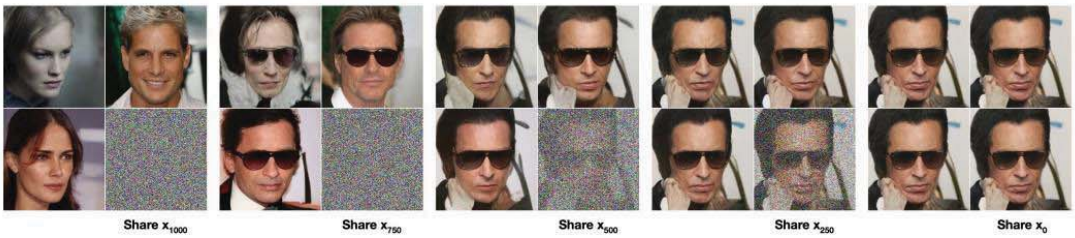

Figure 7: When conditioned on the same latent, CelebA-HQ 256×256 samples share high-level attributes. Bottom-right quadrants are $\mathbf{x}_t$, and other quadrants are samples from $p_\theta(\mathbf{x}_0|\mathbf{x}_t)$.

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Figure 8: Interpolations of CelebA-HQ 256x256 images with 500 timesteps of diffusion.

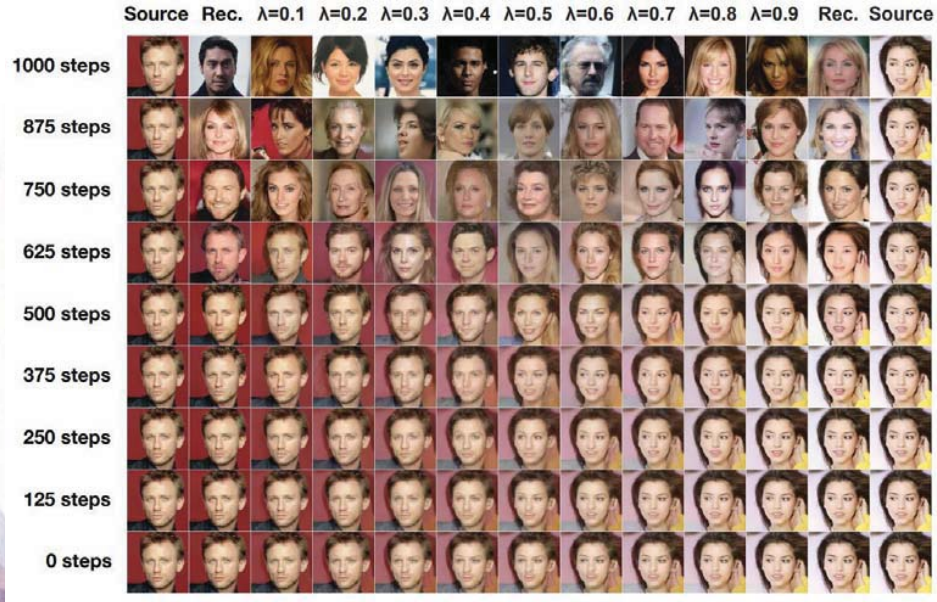

Figure 9: Coarse-to-fine interpolations that vary the number of diffusion steps prior to latent mixing.

Classifier-free guidance

$$
\begin{aligned}
\nabla_{\mathbf{x}_t} \log p(y|\mathbf{x}_t) &= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|y) - \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t) \\
&= -\frac{1}{\sqrt{1-\bar{\alpha}_t}} \Big(\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \Big) \\
\bar{\boldsymbol{\epsilon}}_\theta(\mathbf{x}_t, t, y) &= \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - \sqrt{1-\bar{\alpha}_t}\, w \nabla_{\mathbf{x}_t} \log p(y|\mathbf{x}_t) \\
&= \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) + w\big(\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\big) \\
&= (w+1)\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - w\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)
\end{aligned}
$$

Summary

Diffusion and Construction of Global Flow

Inference with Gaussians

Learning in DDPM

KSBI | 한국생명정보학회

KSBi-BIML 2024

Diffusion Models - 이해와 응용

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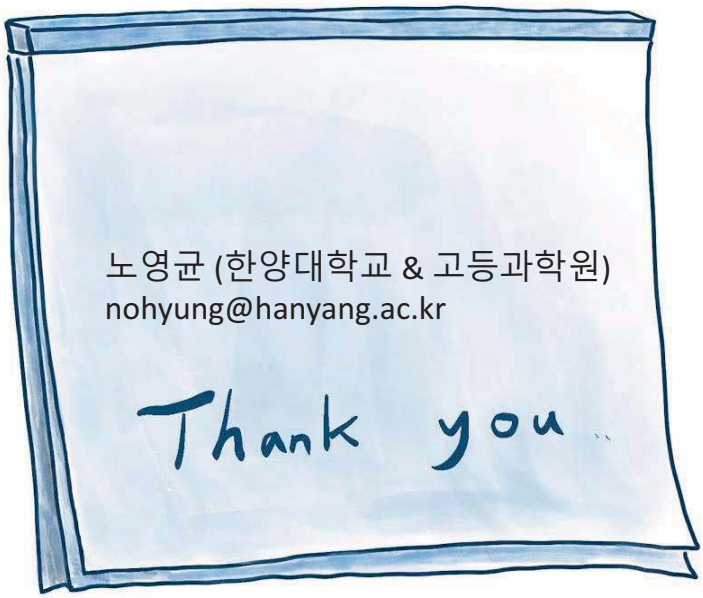
Link

CoLab -> Open notebook -> Github ->

Enter a GitHub URL or search by organization or user
nohyung

Repository
nohyung/2024_BIML



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