Diffusion Models

2024 Machine Learning Algorithms class

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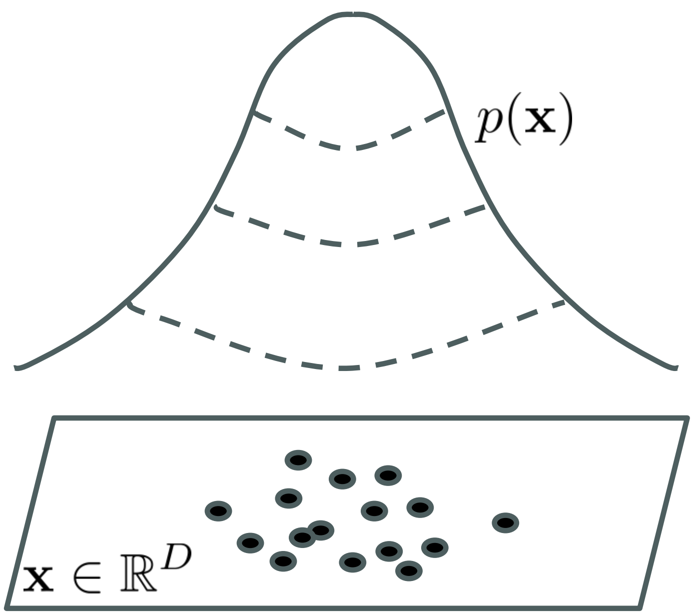
Data Generation

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



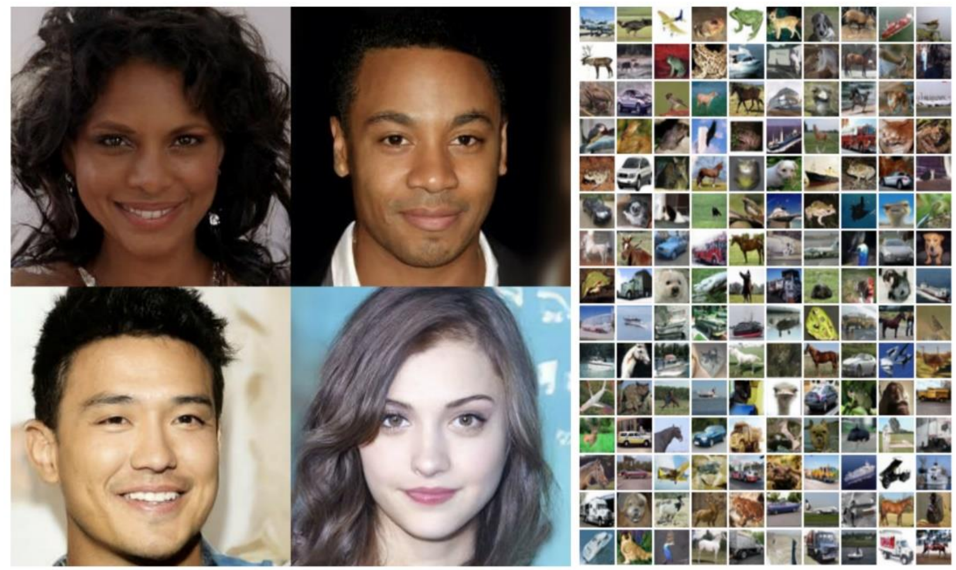


Figure 1: Generated samples on CelebA-HQ 256×256 (left) and unconditional CIFAR10 (right)

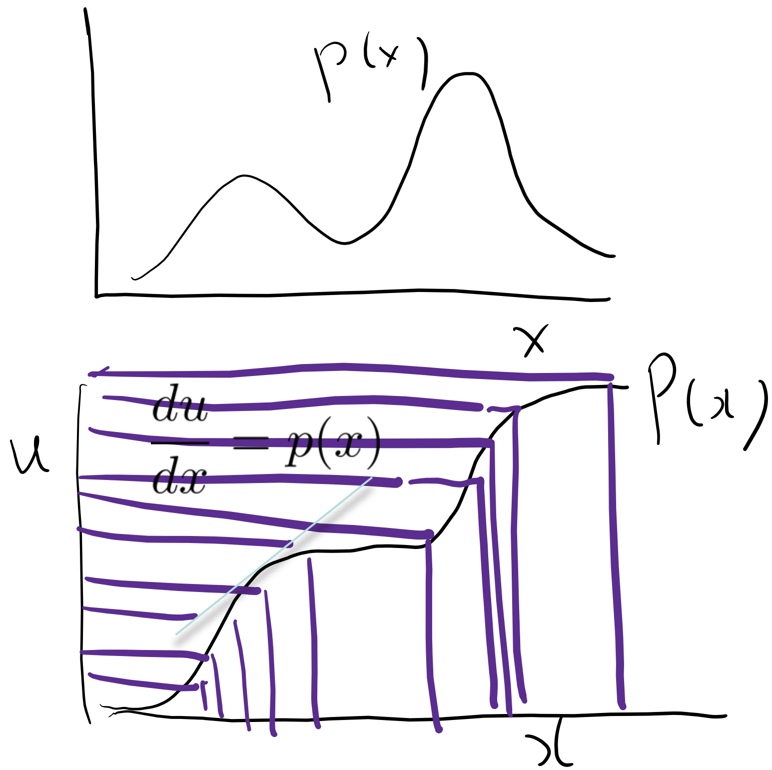
$$\mathbf{x} \in \mathbb{R}^{\text{Pixel}}$$

Data Generation 101

Cumulative distribution

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

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



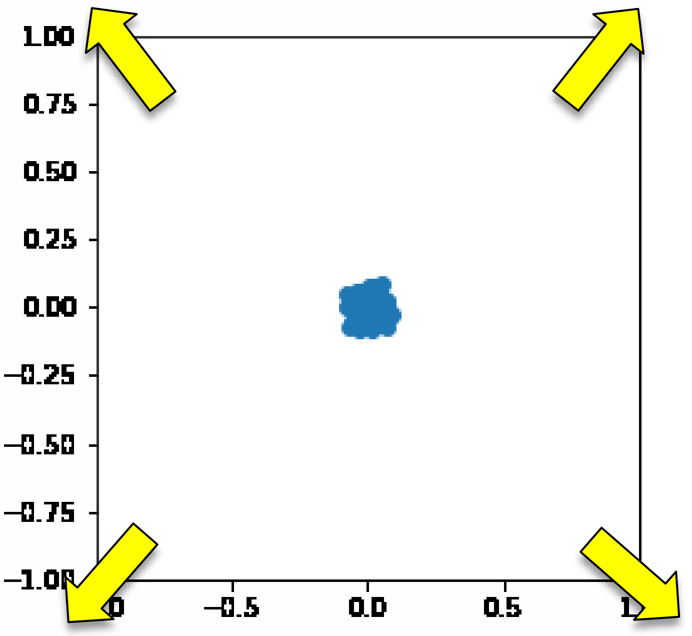
$$\frac{du}{dx} = p(x)$$

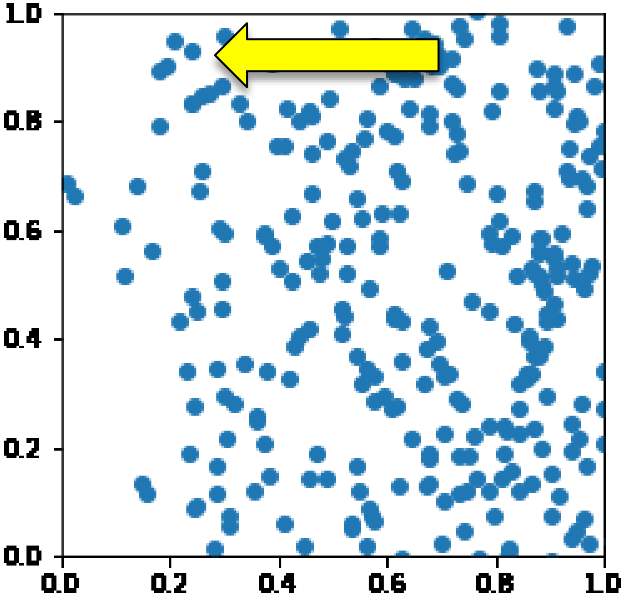
$$du = p(x)dx$$

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

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

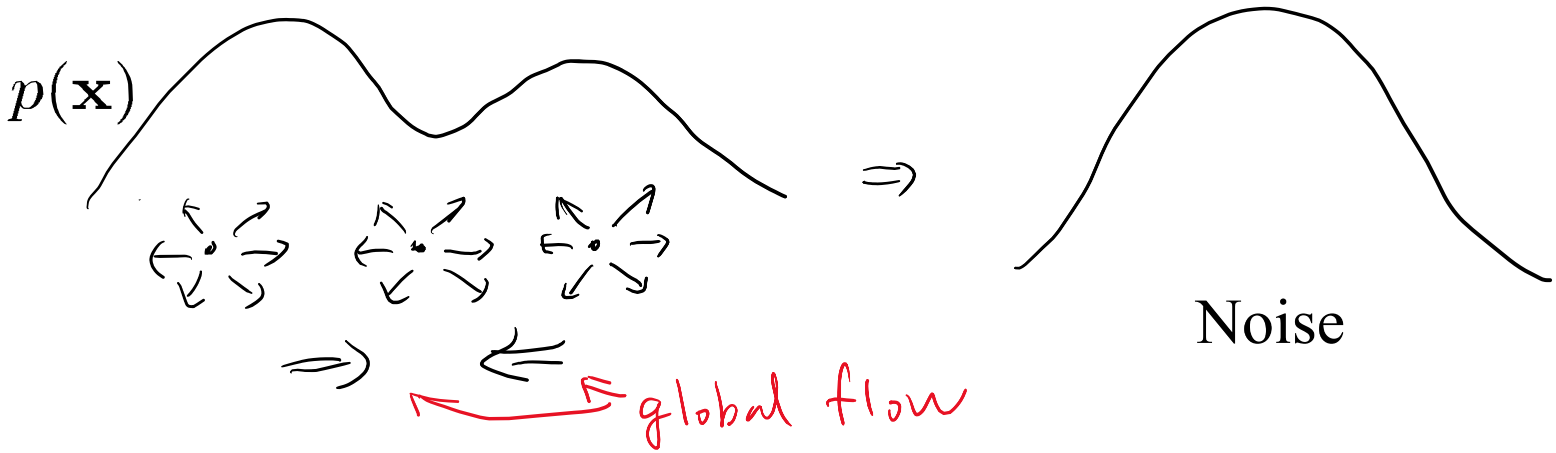
Diffusion


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−0.5
0.0
0.5

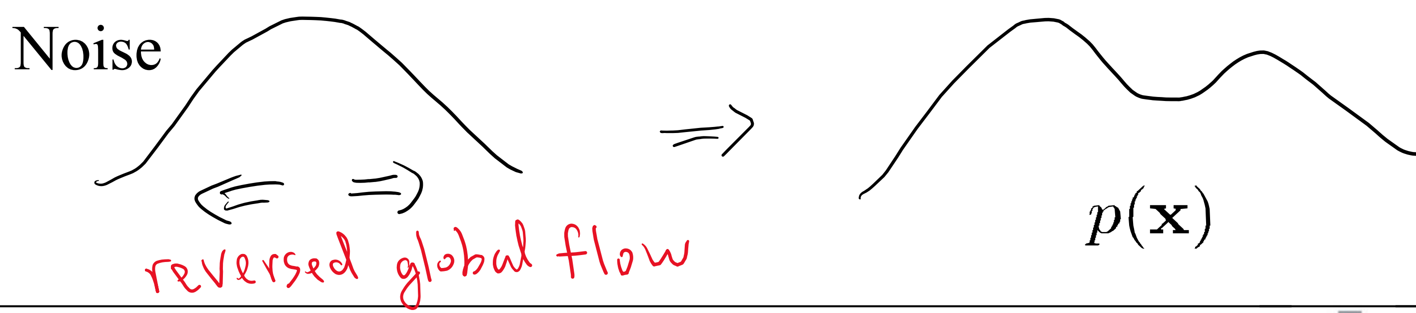

1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0

Diffusion of Non-Uniform Density

- Diffusion of Non-uniform density makes a global flow



- Reverse process in diffusion model reconstructs the backward global flow.



Denoising Diffusion Probabilistic Models

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Abstract

We present high quality image synthesis results using diffusion probabilistic models, a class of latent variable models inspired by considerations from nonequilibrium thermodynamics. Our best results are obtained by training on a weighted variational bound designed according to a novel connection between diffusion probabilistic models and denoising score matching with Langevin dynamics, and our models naturally admit a progressive lossy decompression scheme that can be interpreted as a generalization of autoregressive decoding. On the unconditional CIFAR10 dataset, we obtain an Inception score of 9.46 and a state-of-the-art FID score of 3.17. On 256x256 LSUN, we obtain sample quality similar to ProgressiveGAN. Our imple-

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Diffussion Models

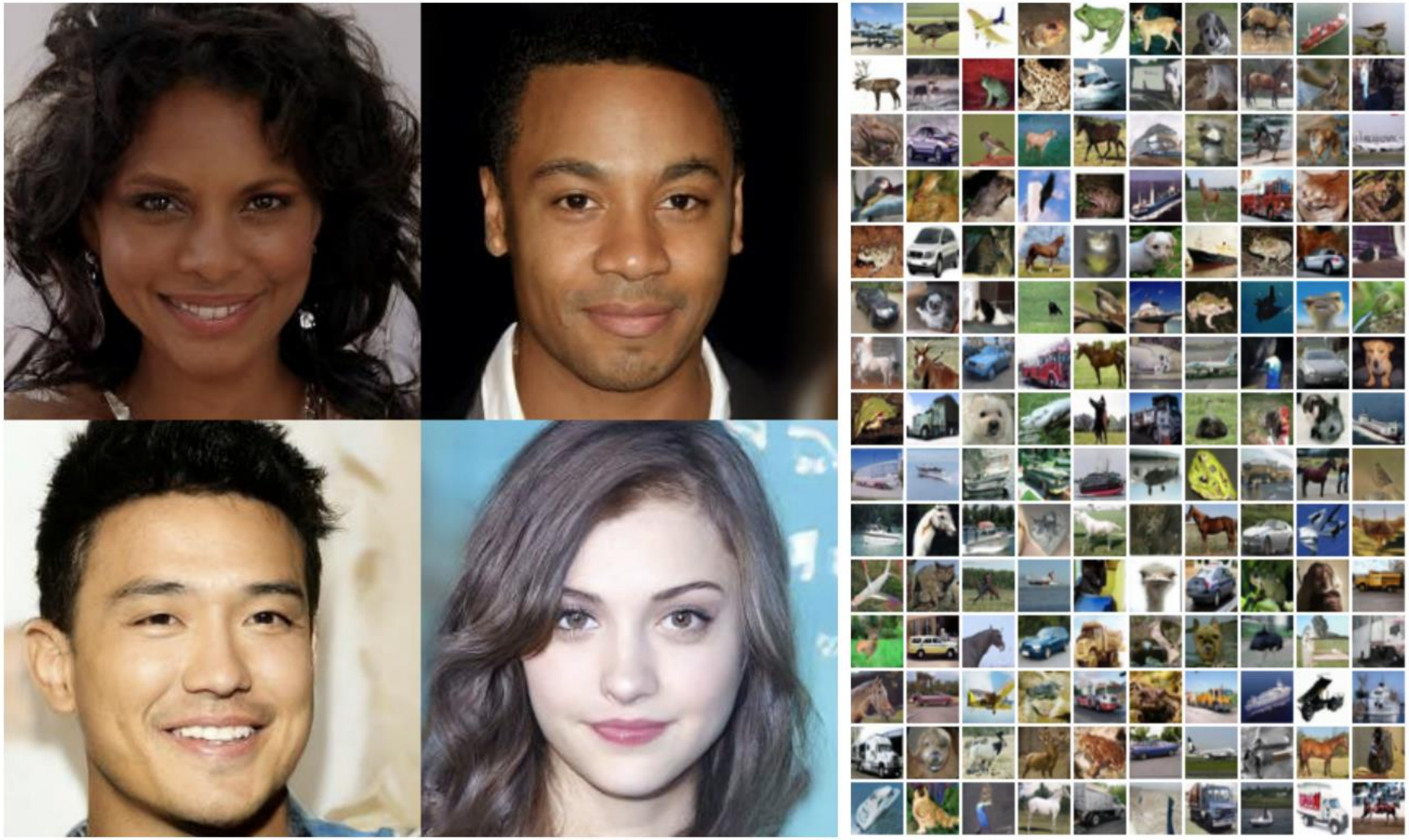


Figure 1: Generated samples on CelebA-HQ 256×256 (left) and unconditional CIFAR10 (right)

Underlying Dffusion Procedure

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

Data

$$\mathbf{x}_0 \sim q(\mathbf{x}_0)$$

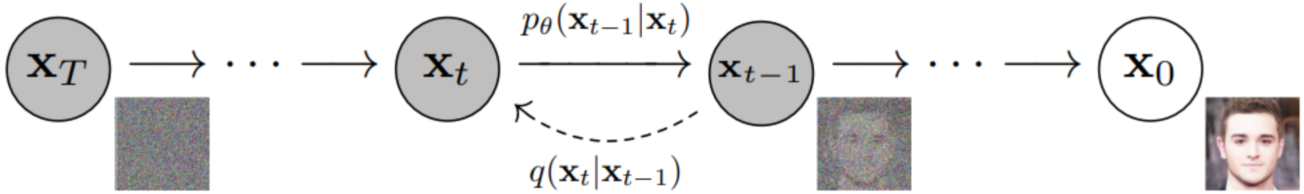


Figure 2: The directed graphical model considered in this work.

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

$\beta_t > 0$

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

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

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

: Gaussian mixture

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

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:

$$\begin{aligned}\mathbb{E}\left[-\log p_\theta(\mathbf{x}_0)\right] &\leq \mathbb{E}_q\left[-\log\frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] \\ &= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1}\log\frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] =: L\end{aligned}$$

Look at the derivations in the next two pages…

Constructing Objective Functions - 1

$$
\begin{aligned}
L &= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1}\log\frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] \\
&= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1}\log\frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t)}\cdot\frac{q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)}\right] \\
&= \mathbb{E}_q\left[-\log\frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T)} - \sum_{t\geq 1}\log\frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t)} - \log q(\mathbf{x}_0)\right] \\
&= D_{\mathrm{KL}}(q(\mathbf{x}_T)\,\|\,p(\mathbf{x}_T)) + \mathbb{E}_q\left[\sum_{t\geq 1} D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t)\,\|\,p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))\right] + H(\mathbf{x}_0)
\end{aligned}
$$

Can we have this density function?

Constructing Objective Functions - 2

$$
\begin{aligned}
L &= \mathbb{E}_q\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] \\
&= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] \\
&= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t>1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} - \log \frac{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_1|\mathbf{x}_0)}\right] \\
&= \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t>1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} \cdot \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} - \log \frac{p_\theta(\mathbf{x}_0|\mathbf{x}_1)}{q(\mathbf{x}_1|\mathbf{x}_0)}\right] \\
&= \mathbb{E}_q\left[-\log \frac{p(\mathbf{x}_T)}{q(\mathbf{x}_T|\mathbf{x}_0)} - \sum_{t>1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)} - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)\right]
\end{aligned}
$$

Gaussians

$\because$ x_0 given

$$
= \mathbb{E}_q\Big[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \,\|\, p(\mathbf{x}_T))}_{L_T} + \underbrace{\sum_{t>1} D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \,\|\, p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\Big] \quad (22)
$$

Tractable Functions

$$\left.\begin{array}{c} q(\mathbf{x}_{t-1}|\mathbf{x}_0) \\ q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) \\ q(\mathbf{x}_t|\mathbf{x}_0) \end{array}\right\}\ \text{Gaussians}$$

Decomposition for Gaussian Inference

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

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

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

Decomposition for Gaussian Inference

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

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

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

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

$$\Sigma_{a|b} = \Sigma_a - \Sigma_{ab}\Sigma_b^{-1}\Sigma_{ba}$$

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

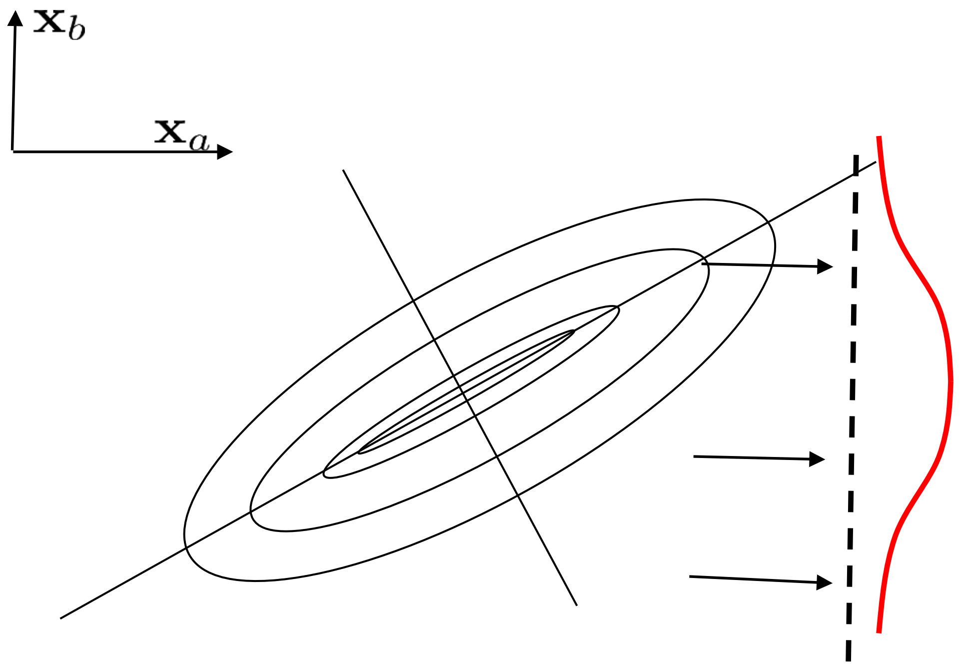
Decomposition for Inference

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

$$\begin{aligned} p(\mathbf{x}) &= \frac{1}{\sqrt{2\pi}^D |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2} (\mathbf{x}-\mu)^\top \Sigma^{-1} (\mathbf{x}-\mu) \right) \\ &= C_1 \exp\left(-\frac{1}{2} (\mathbf{x}_a - \mu_{a|b}(\mathbf{x}_b))^\top \Sigma_{a|b}^{-1} (\mathbf{x}_a - \mu_{a|b}(\mathbf{x}_b)) \right) \cdot \\ &\qquad C_2 \exp\left(-\frac{1}{2} (\mathbf{x}_b - \mu_b)^\top \Sigma_b^{-1} (\mathbf{x}_b - \mu_b) \right) \end{aligned}$$

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

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 – Marginal

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

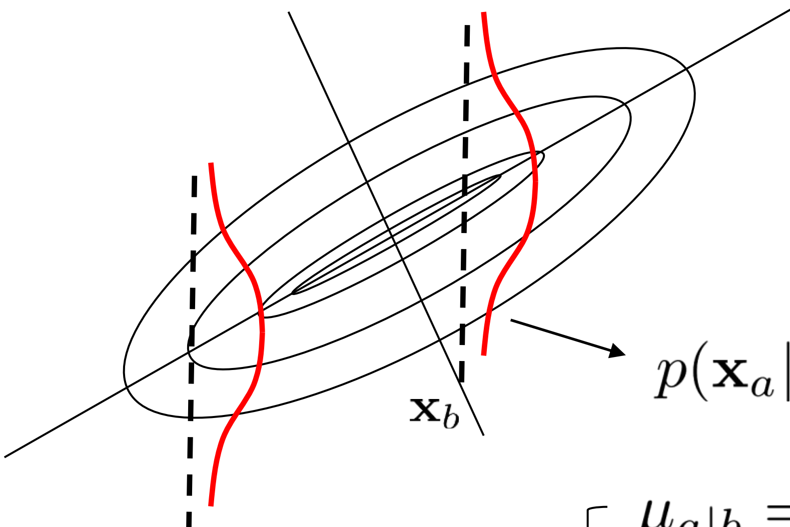
$$p(\mathbf{x}_a, \mathbf{x}_b) = \frac{1}{\sqrt{2\pi}^{D}\left|\begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b \end{pmatrix}\right|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}\begin{pmatrix} \mathbf{x}_a-\mu_a \\ \mathbf{x}_b-\mu_b \end{pmatrix}^\top \begin{pmatrix} \Sigma_a & \Sigma_{ab}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

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

$$= \mathcal{N}(\mu_a, \Sigma_a)$$

Gaussian Random Variable – Conditioning

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

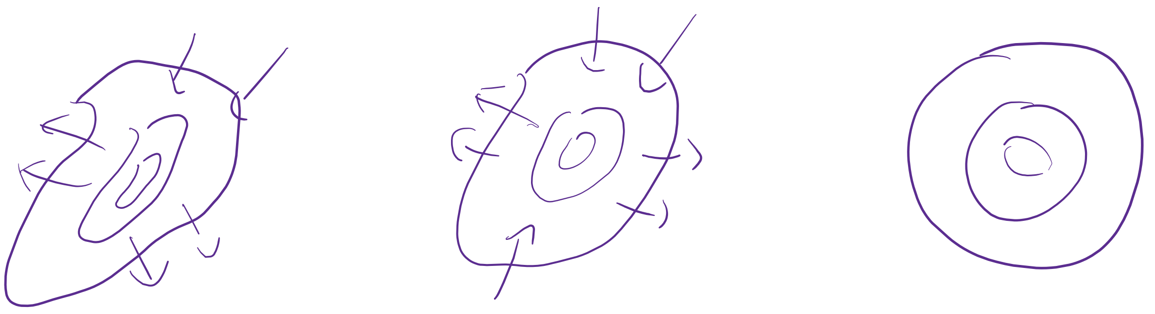


$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix} \quad \begin{matrix} \mathbf{x}_a \in \mathbb{R}^{D_a} \\ \mathbf{x}_b \in \mathbb{R}^{D_b} \end{matrix}$$

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

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

Diffusion and Reverse Process



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

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

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

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

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

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

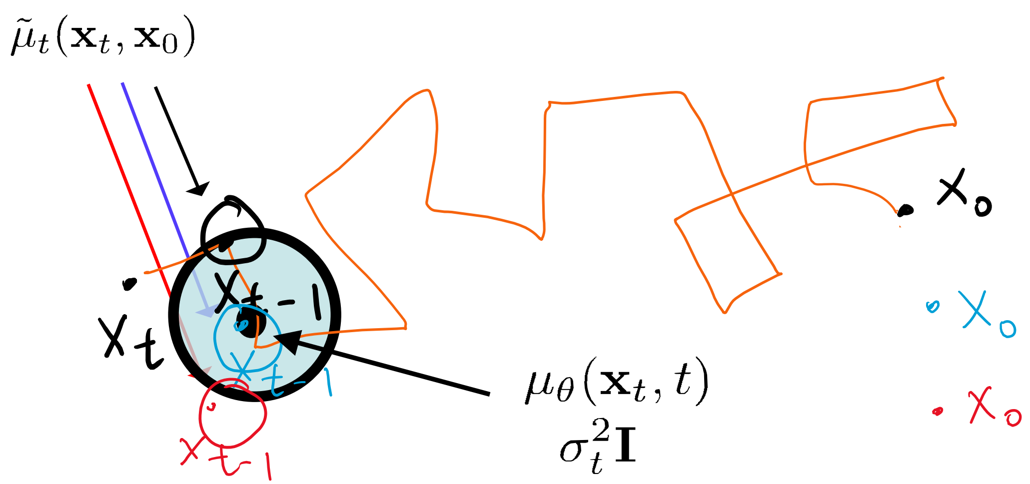
$$\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t,\mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t \quad \text{and} \quad \tilde{\beta}_t := \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$$

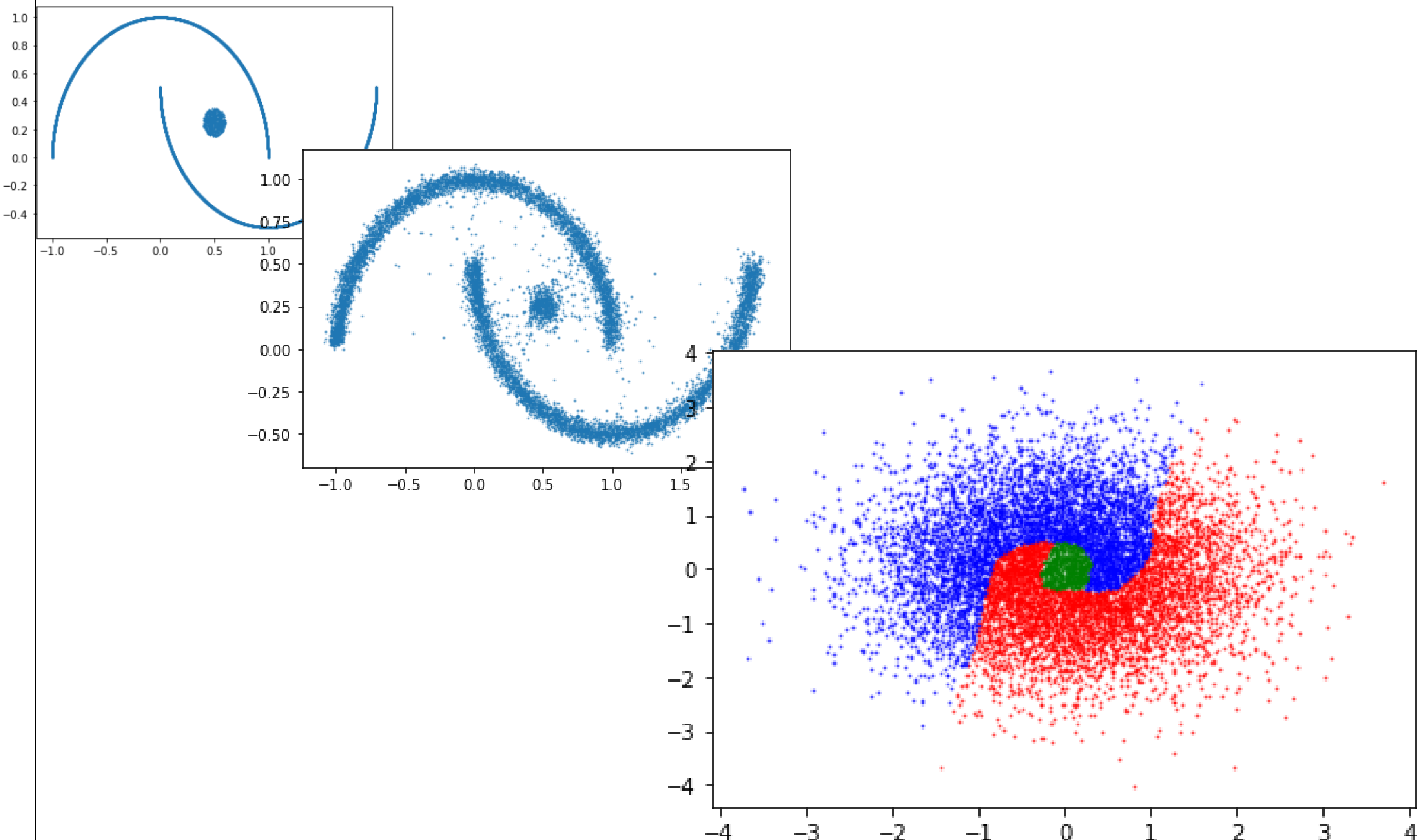
- Model

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

- K-L divergence:

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




1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−1.0
−0.5
0.0
0.5
1.0
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−1.0
−0.5
0.0
0.5
1.0
1.5
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

Conditional Mean

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

$$L_{t-1} - C$$

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

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

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 $\mathbf{x}_t$

- New parameterization

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

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

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

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

Learning without Generating $x_{1,}$ $x_{2,}$ …, x_{t-1}

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

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

Algorithm 1 Training

1: **repeat**

2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$

3: $t \sim \text{Uniform}(\{1, \ldots, T\})$

4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

5: Take gradient descent step on

$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}}_{= \mathbf{x}_t}, t) \right\|^2$$

6: **until** converged

Algorithm 2 Sampling

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

Results

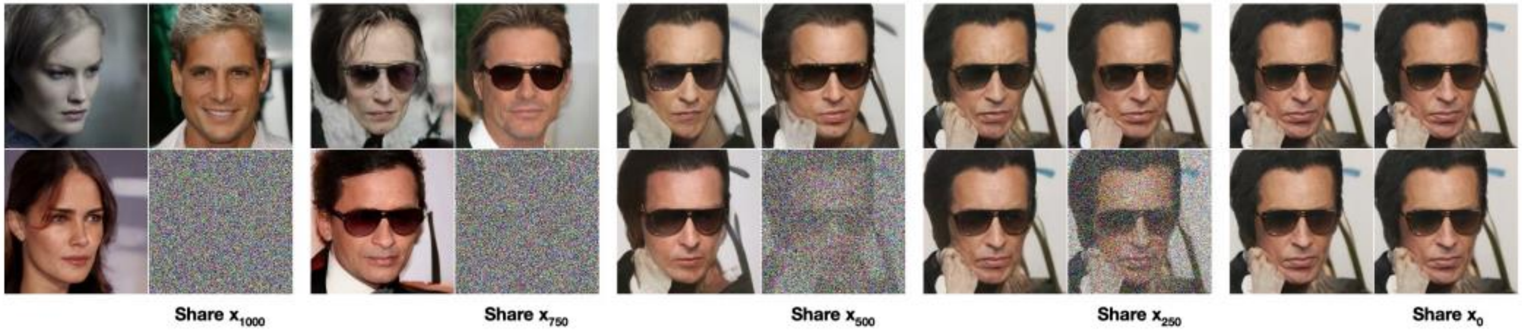


Figure 7: When conditioned on the same latent, CelebA-HQ 256 × 256 samples share high-level attributes. Bottom-right quadrants are $\mathbf{x}_t$, and other quadrants are samples from $p_\theta(\mathbf{x}_0|\mathbf{x}_t)$.

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

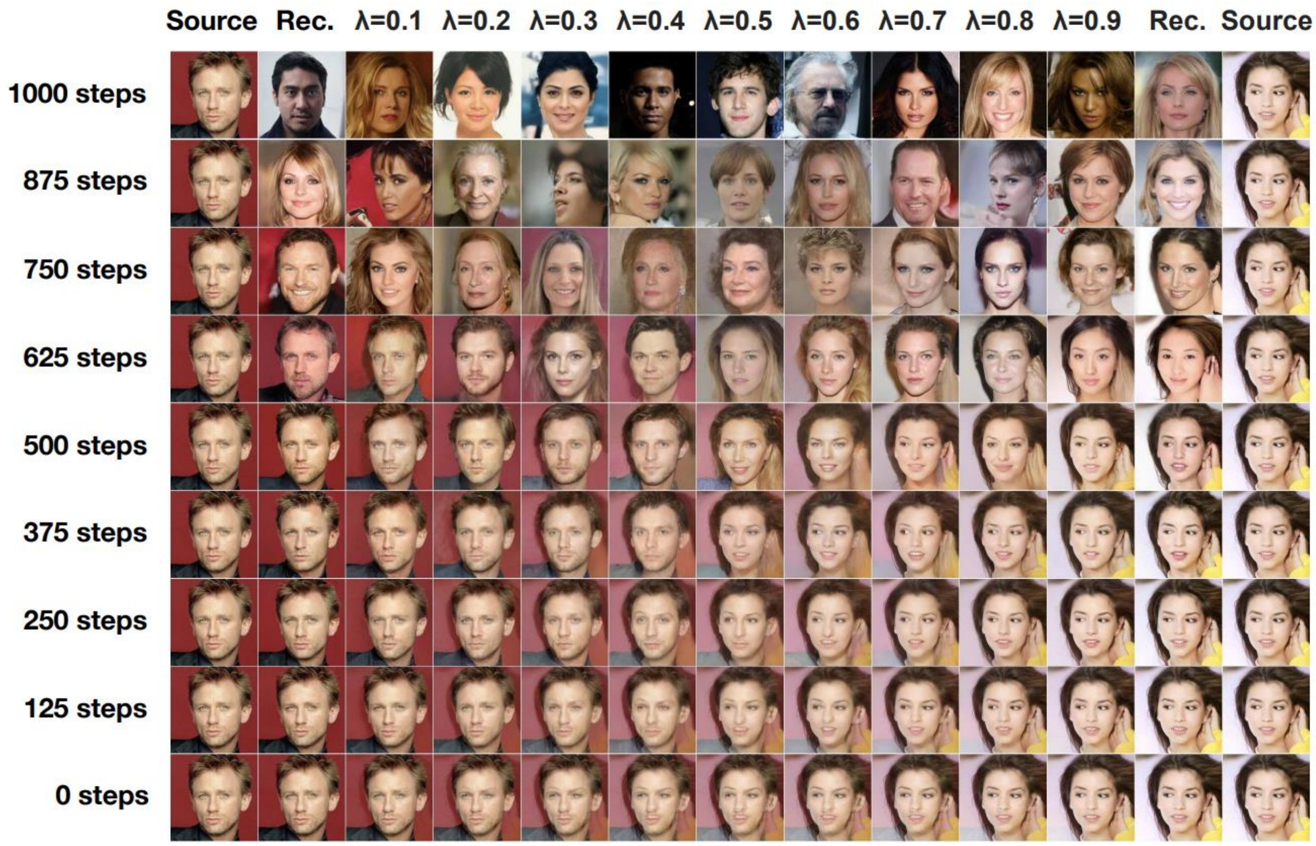


Figure 9: Coarse-to-fine interpolations that vary the number of diffusion steps prior to latent mixing.

Classifier-free Guidance

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

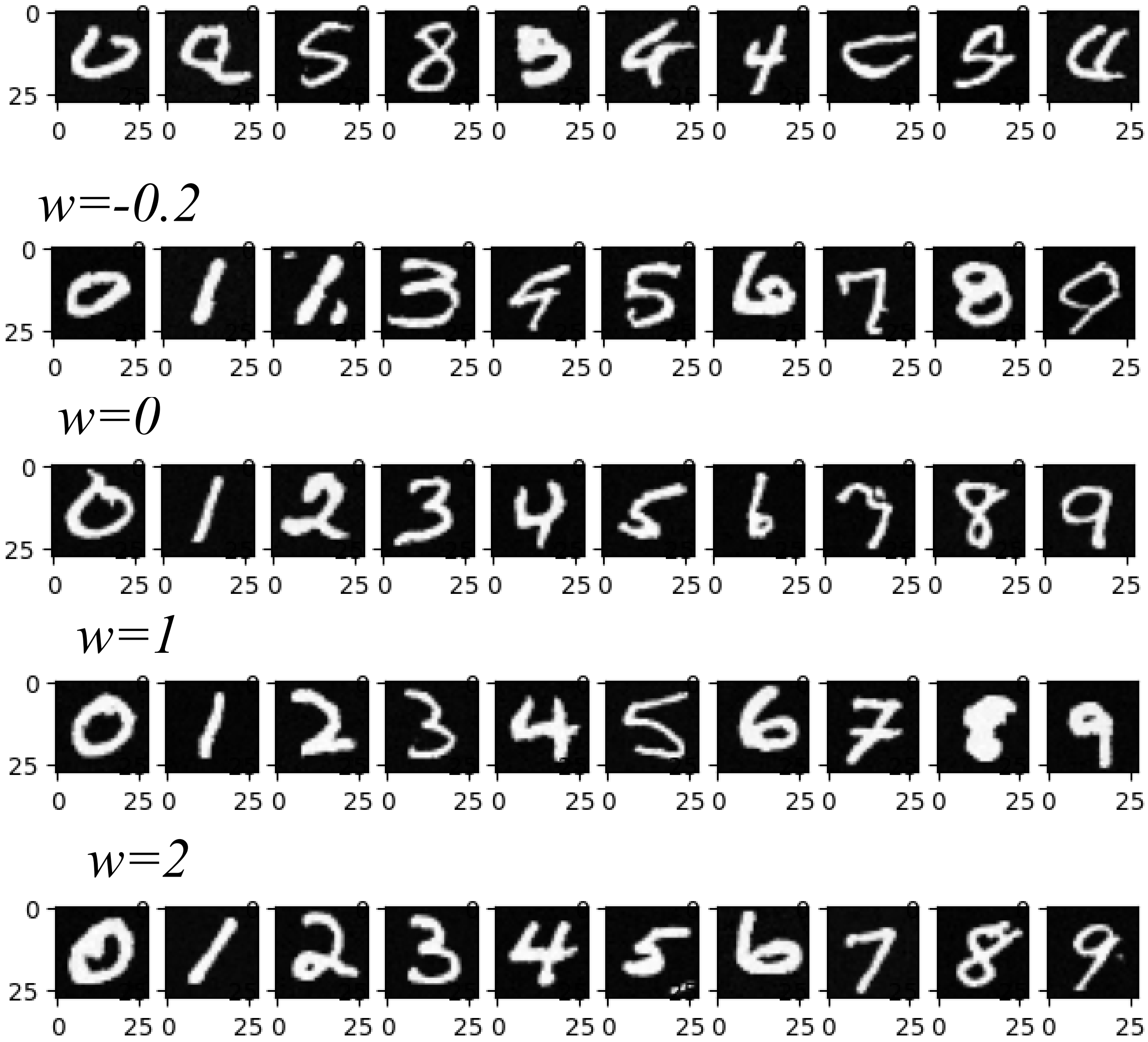
w=-1

w=-0.2

w=0

w=1

w=2



https://github.com/nohyung/2024_Diffusion_models/blob/main/Diffusion_MNIST_Noh_example.ipynb

Summary

- Diffusion and Construction of Global Flow
- Inference with Gaussians
- Learning in DDPM and classifier-free guidance


Thank you ..