Elucidating the Exposure Bias in Diffusion Models

ICLR, 2024

Miao's Group - Paper Reading

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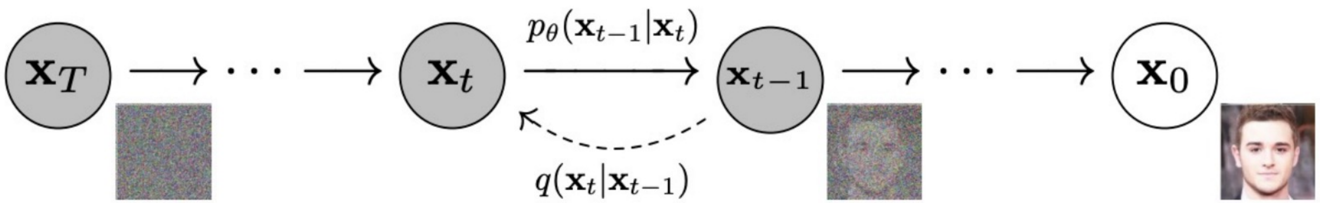
时间：2024.4.9

Recall Denoising Diffusion Probability Models

Recall Denoising Diffusion Probability Models



$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t \boldsymbol{I})$$

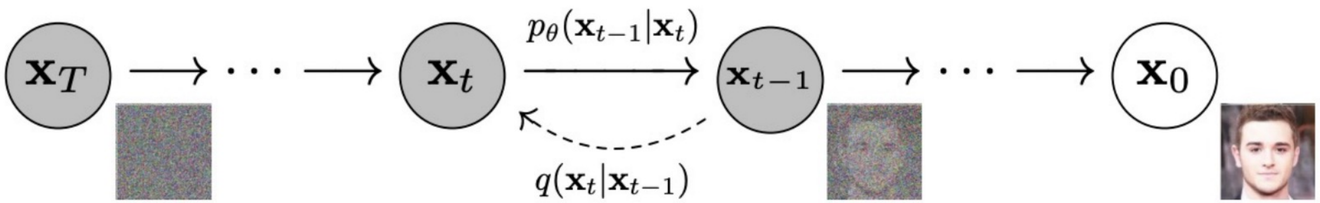
$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \boldsymbol{I})$$

$$\tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$$

$$\tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t$$

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

Recall Denoising Diffusion Probability Models



$$\alpha_t = 1 - \beta_t, \bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

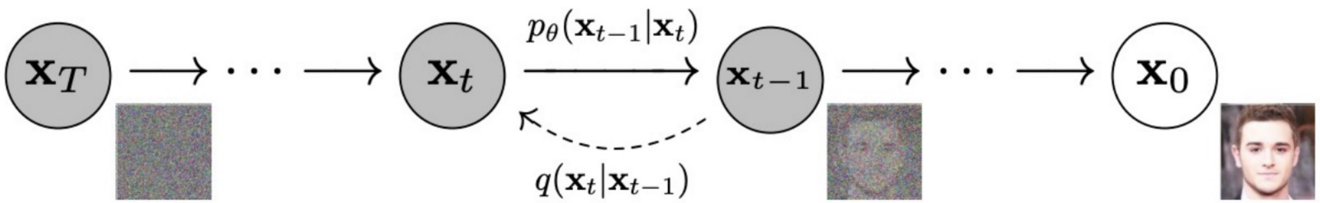
$$\begin{aligned}
\mathbf{x}_t &= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} \\
&= \sqrt{\alpha_t \alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_t \alpha_{t-1}}\bar{\boldsymbol{\epsilon}}_{t-2} \\
&= \cdots \\
&= \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}
\end{aligned}$$

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

Algorithm 1 Training

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

Recall Denoising Diffusion Probability Models



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

$$\tilde{\mu}(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$$

$$\tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t$$

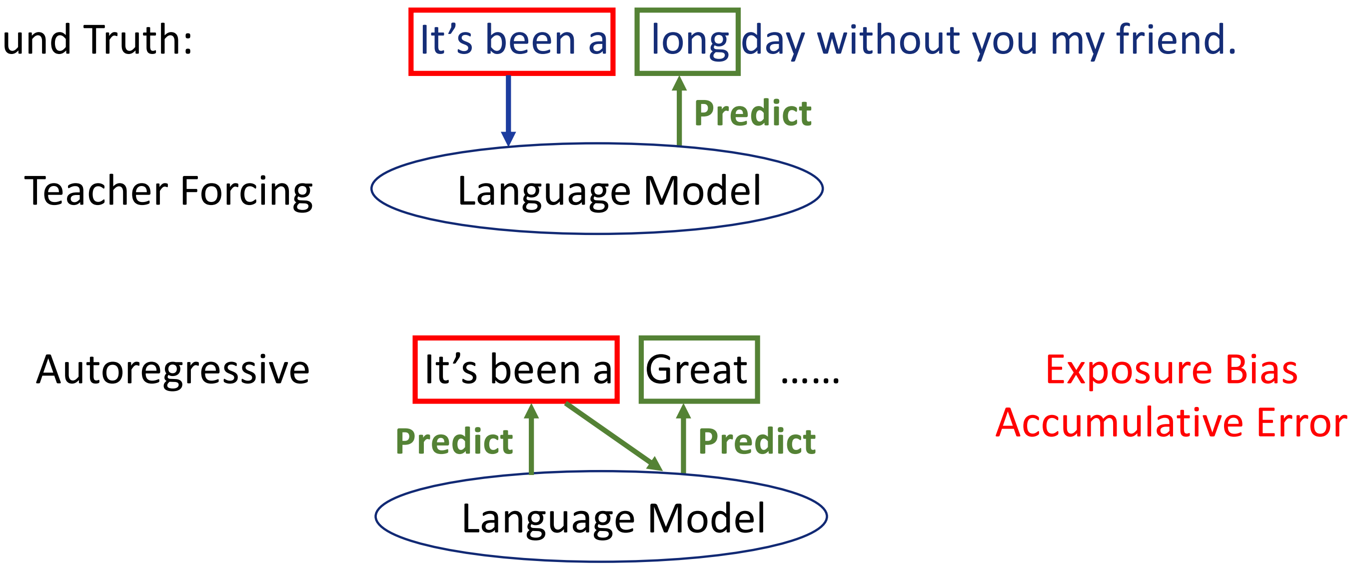
Algorithm 2 Sampling

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** $\mathbf{x}_0$

Elucidating the Exposure Bias in Diffusion Models

Elucidating the Exposure Bias in Diffusion Models

- What is Exposure Bias?
  - Example: Train a Language Model
  - Ground Truth:



Elucidating the Exposure Bias in Diffusion Models

- Exposure Bias in Diffusion Models

Algorithm 1 Training

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

Algorithm 2 Sampling

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

Teacher Forcing

Exposure Bias
Accumulative Error

Elucidating the Exposure Bias in Diffusion Models

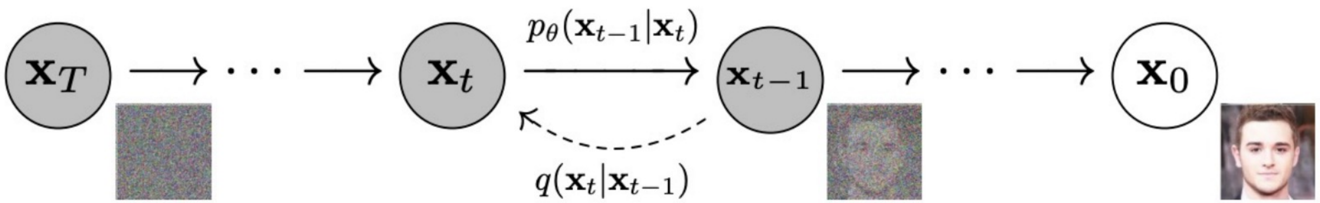
- Exposure Bias in Diffusion Models

Sampling Distribution	Training Distribution
$q\left(\hat{\mathbf{x}}_t \middle| \mathbf{x}_{t+1}, \mathbf{x}_\theta^{t+1}\right)$	$q(\mathbf{x}_t \mid \mathbf{x}_0)$
采样阶段看到的 $\hat{\mathbf{x}}_t$	训练时在时间步 t 看到的 $\mathbf{x}_t$

接下来看 $\hat{\mathbf{x}}_t$ 和 $\mathbf{x}_t$ 的区别

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

Elucidating the Exposure Bias in Diffusion Models



$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t \boldsymbol{I})$$

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

$$\tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right) \qquad \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\cdot\beta_t$$

$$\mathbf{x}_\theta^t$$

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

Elucidating the Exposure Bias in Diffusion Models

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

$$\tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$$

$\mathbf{x}_\theta^t$

Sampling: $\mathbf{x}_\theta^t - \mathbf{x}_0 \neq 0$

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

Elucidating the Exposure Bias in Diffusion Models

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

$$\tilde{\boldsymbol{\mu}}(\mathbf{x}_t,\mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$$

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

$$\mathbf{x}_\theta^t$$

Modeling

$$p_\theta(\mathbf{x}_0|\mathbf{x}_t) = \mathcal{N}\left(\mathbf{x}_\theta^t; \mathbf{x}_0, e_t^2 \boldsymbol{I}\right), \qquad \mathbf{x}_\theta^t = \mathbf{x}_0 + e_t\epsilon_0 \left(\epsilon_0 \sim \mathcal{N}(0,I)\right)$$

$$\hat{\mathbf{x}}_t = \frac{\sqrt{\bar{\alpha}_t}\beta_{t+1}}{1-\bar{\alpha}_{t+1}}\mathbf{x}_\theta^{t+1} + \frac{\sqrt{\bar{\alpha}_{t+1}}(1-\bar{\alpha}_t)}{1-\bar{\alpha}_{t+1}}\mathbf{x}_{t+1} + \sqrt{\tilde{\beta}_{t+1}}\epsilon_1$$

$$\hat{\mathbf{x}}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t + \left(\frac{\sqrt{\bar{\alpha}_t}\beta_{t+1}}{1-\bar{\alpha}_{t+1}}e_{t+1}\right)^2}\,\epsilon_3$$

Elucidating the Exposure Bias in Diffusion Models

- Exposure Bias in Diffusion Models

Training Distribution	Sampling Distribution
$q(\mathbf{x}_t \vert \mathbf{x}_0)$	$q(\hat{\mathbf{x}}_t \vert \mathbf{x}_{t+1}, \mathbf{x}_\theta^{t+1})$
训练时在时间步 t 看到的 $\mathbf{x}_t$	采样阶段看到的 $\hat{\mathbf{x}}_t$
$\mathbf{x}_{\mathrm{t}} = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$	$\hat{\mathbf{x}}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t + \left(\frac{\sqrt{\bar{\alpha}_t}\beta_{t+1}}{1-\bar{\alpha}_{t+1}} e_{t+1}\right)^2}\boldsymbol{\epsilon}_3$

mean	$\sqrt{\bar{\alpha}_t}\mathbf{x}_0$	$\sqrt{\bar{\alpha}_t}\mathbf{x}_0$
variance	$(1-\bar{\alpha}_t)\boldsymbol{I}$	$\left(1-\bar{\alpha}_t + \left(\frac{\sqrt{\bar{\alpha}_t}\beta_{t+1}}{1-\bar{\alpha}_{t+1}} e_{t+1}\right)^2\right)\boldsymbol{I}$ bigger!

Elucidating the Exposure Bias in Diffusion Models

- Exposure Bias in Diffusion Models

Training Distribution

$$\mathbf{x}_\mathrm{t} = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$$

Sampling Distribution

bigger!

$$\hat{\mathbf{x}}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t + \left(\frac{\sqrt{\bar{\alpha}_t}\beta_{t+1}}{1-\bar{\alpha}_{t+1}} e_{t+1}\right)^2}\,\boldsymbol{\epsilon}_3$$

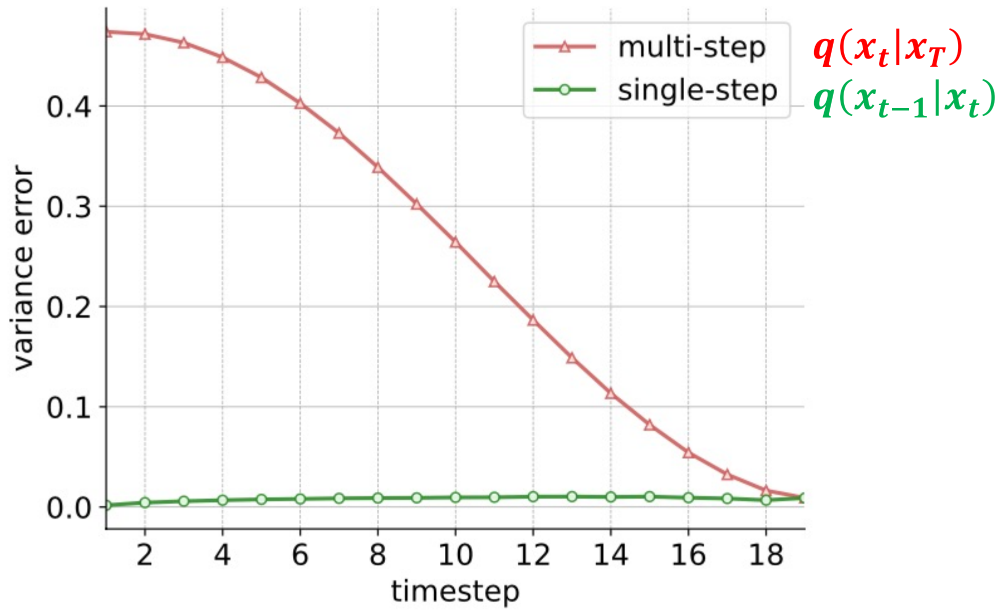


Figure 1: Variance error in single-step and multi-step samplings.

Elucidating the Exposure Bias in Diffusion Models

- Exposure Bias in Diffusion Models

Training Distribution

$$\boxed{\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}}$$

Sampling Distribution

bigger!

$$\boxed{\hat{\mathbf{x}}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t + \left(\frac{\sqrt{\bar{\alpha}_t}\beta_{t+1}}{1-\bar{\alpha}_{t+1}} e_{t+1}\right)^2}\,\boldsymbol{\epsilon}_3}$$

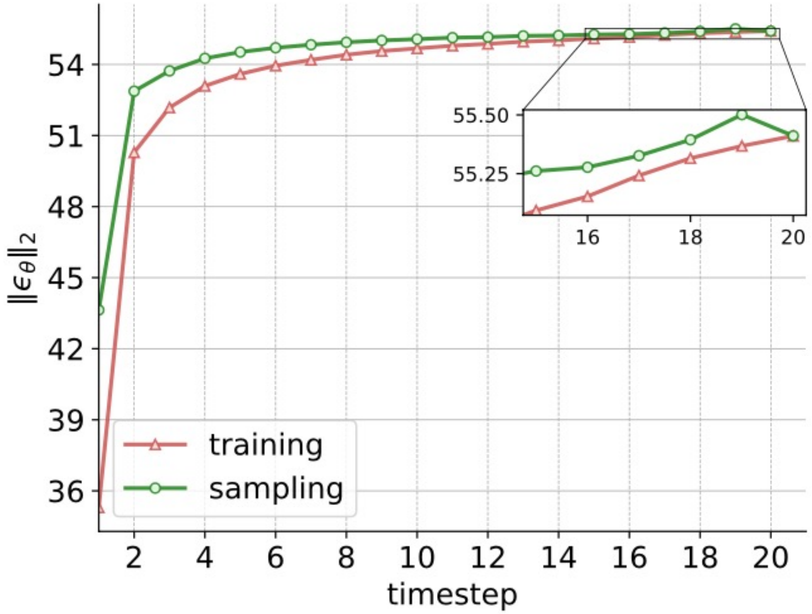


Figure 2: $\|\boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\cdot)\|_2$ during training and sampling on CIFAR-10. We use 20-step sampling and report the L2-norm using 50k samples at each timestep.

Elucidating the Exposure Bias in Diffusion Models

- Exposure Bias in Diffusion Models

Training Distribution

$$\boxed{\mathbf{x}_{\mathrm{t}} = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}}$$

Sampling Distribution

bigger!

$$\boxed{\hat{\mathbf{x}}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t + \left(\frac{\sqrt{\bar{\alpha}_t}\beta_{t+1}}{1-\bar{\alpha}_{t+1}}e_{t+1}\right)^2}\,\boldsymbol{\epsilon}_3}$$

Solution

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: $\quad \mathbf{x}_{t-1} = \boxed{\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)} + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

$$\tilde{\mu}(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\frac{\boldsymbol{\epsilon}_t}{\lambda_t}\right)$$

Elucidating the Exposure Bias in Diffusion Models

- Result

T'	Model	Unconditional			Conditional	
		CIFAR-10 32×32	LSUN 64×64	FFHQ 128×128	ImageNet 64×64	ImageNet 128×128
100	ADM	3.37	3.59	14.52	2.71	3.55
	ADM-ES	**2.17**	**2.91**	**6.77**	**2.39**	**3.37**
50	ADM	4.43	7.28	26.15	3.75	5.15
	ADM-ES	**2.49**	**3.68**	**9.50**	**3.07**	**4.33**
20	ADM	10.36	23.92	59.35	10.96	12.48
	ADM-ES	5.15	8.22	26.14	7.52	9.95
	ADM-ES*	**4.31**	**7.60**	**24.83**	**7.37**	**9.86**

Elucidating the Exposure Bias in Diffusion Models

- Result

T'	Model	Unconditional		Conditional	
		Heun	Euler	Heun	Euler
35	EDM	1.97	3.81	1.82	3.74
	EDM-ES (ours)	**1.95**	**2.80**	**1.80**	**2.59**
21	EDM	2.33	6.29	2.17	5.91
	EDM-ES	**2.24**	**4.32**	**2.08**	**3.74**
13	EDM	7.16	12.28	6.69	10.66
	EDM-ES	**6.54**	**8.39**	**6.16**	**6.59**

Reference

- What are Diffusion Models? | Lil'Log (lilianweng.github.io)
- Ho, Jonathan, Ajay Jain, and Pieter Abbeel. "Denoising diffusion probabilistic models." NIPS 2020
- Mang Ning, Mingxiao Li, Jianlin Su, Albert Ali Salah, Itir Önal Ertugrul. "Elucidating the Exposure Bias in Diffusion Models" ICLR 2024

Q&A

Thanks

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