Bias Mitigation in Graph Diffusion Models

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Those who wish to succeed must ask the right preliminary questions. —Aristotle

Bias Mitigation in Graph Diffusion Models

Graph Diffusion models

- Given the constraints of graph data scale and network learning capacity, these models truncate the forward diffusion process to enhance performance, preventing it from fully reaching the standard Gaussian distribution.
- However, during sampling, they have to start from the standard Gaussian distribution without employing any specific strategy.
- This mismatch is a critical issue and including exposure bias.

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Graph diffusion models

Model Dataset	GDSS Comm.	GSDM Enz	HGDM QM9	MOOD ZINC250k
Type	Edge	Eigen	Edge	Node
SDE	VPSDE	VPSDE	VESDE	VPSDE
$\beta_{\min}\|\sigma_{\min}$	0.1	0.1	0.1	0.1
$\beta_{\max}\|\sigma_{\max}$	1.0	1.0	1.0	1.0
u_T	0.7596	0.7596	1.0	0.7596
σ_T^2	0.4231	0.4231	1.0	0.4231

Figure: (a) starting bias

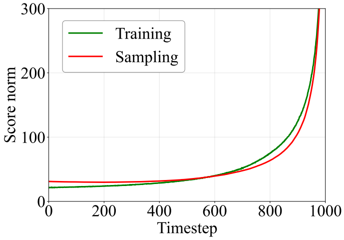

Figure: (b) Baseline

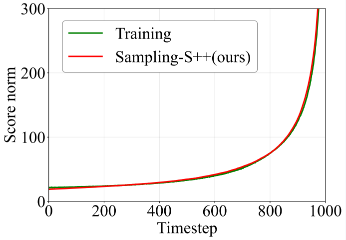

Figure: (c) corrected

$$p(\mathbf{z}_t|\mathbf{x}) = \mathcal{N}\left(\mathbf{z}_t|e^{-\frac{1}{4}t^2(\beta_{\max}-\beta_{\min})-\frac{1}{2}t\beta_{\min}}\mathbf{x}, (1-e^{-\frac{1}{2}t^2(\beta_{\max}-\beta_{\min})-t\beta_{\min}})\mathbf{I}\right) = \mathcal{N}(u_t\mathbf{x}, \sigma_t^2\mathbf{I}).$$

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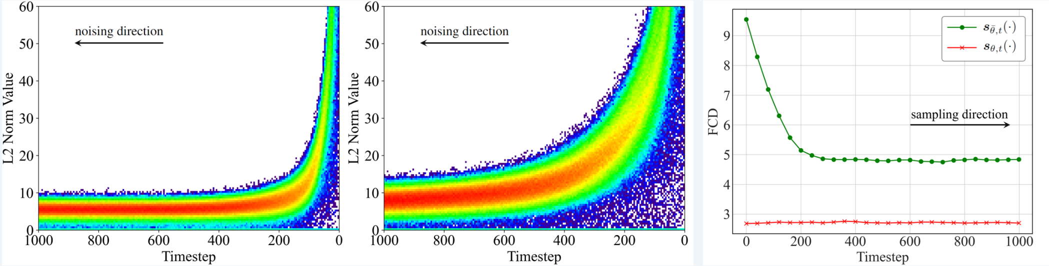
Why baselines are truncated?



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How to correct these bias?

- If we known the inference model $\mathbf{s}(\hat{\mathbf{z}}_t, t, \mathbf{w}^\star)$, and its $\beta_{\min}$ and $\beta_{\max}$, we can use Langevin sampling to correcnt the reverse-starting bias. Moreover, we already have a pretrained score network $\mathbf{s}(\hat{\mathbf{z}}_t, t, \mathbf{w}^\star) \approx \nabla \log p(\mathbf{z}_t|\mathbf{x})$. This score guides Langevin sampling to obtain samples from the distribution $p(\hat{\mathbf{z}}_T) \approx q(\mathbf{z}_T|\mathbf{x})$:

$$\hat{\mathbf{z}}_T = \hat{\mathbf{z}}_T + \gamma \mathbf{s}(\hat{\mathbf{z}}_T, T, \mathbf{w}^\star) + \sqrt{2\gamma}\boldsymbol{\epsilon}$$

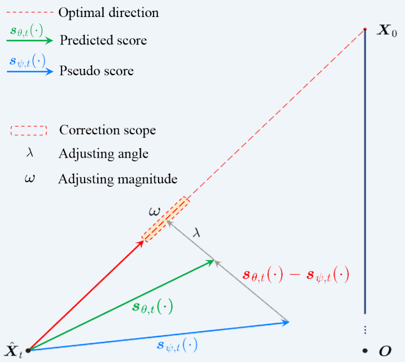
  Here, we use Tweedie formula and have the following equations,

$$\nabla_{\mathbf{z}_t} \log p(\mathbf{z}_t) = -\frac{\boldsymbol{\epsilon}_t}{\sqrt{1-\alpha_t}}$$

$$\mathbf{s} = -\frac{\mathbf{g}}{\sqrt{1-\alpha_t}}$$

Algorithm

$$
\begin{aligned}
&\textbf{for } j = 1 \textbf{ to } M \textbf{ do}\\
&\quad \mathbf{s} = \Big(\mathbf{s} + \lambda(\mathbf{s} - \mathbf{s}(\mathbf{z}_T, \boldsymbol{\psi}^\star, T))\Big)/\omega\\
&\quad \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})\\
&\quad \mathbf{z}_N \leftarrow \mathbf{z}_N + \gamma \mathbf{s} + \sqrt{2\gamma}\boldsymbol{\epsilon}\\
&\textbf{end for}
\end{aligned}
$$



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Ablation

Method	QM9		
	Val. w/o corr. ↑	NSPDK MMD ↓	FCD ↓
GDSS-OC	73.5	0.0157	4.58
GDSS-w/o Correction in sampling	94.8	0.0037	2.65
GDSS-w/o Reverse-starting Alignment	89.8	0.0031	2.01
GDSS-OC-S++	**94.0**	**0.0014**	**1.67**

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Results

Dataset Info.	Community-small Synthetic, $12 \leq \|V\| \leq 20$				Enzymes Real, $10 \leq \|V\| \leq 125$				Grid Synthetic, $100 \leq \|V\| \leq 400$			
Method	Deg.↓	Clus.↓	Orbit↓	Avg.↓	Deg.↓	Clus.↓	Orbit↓	Avg.↓	Deg.↓	Clus.↓	Orbit↓	Avg.↓
GDSS-OC	0.050	0.132	0.011	0.064	0.052	0.627	0.249	0.309	0.270	0.009	0.034	0.070
GDSS-OC-S++	**0.021**	**0.061**	**0.005**	**0.029**	**0.067**	**0.099**	**0.007**	**0.058**	**0.105**	**0.004**	**0.061**	**0.066**
GDSS-WC	0.045	0.088	0.007	0.045	0.044	0.069	0.002	0.038	0.111	0.005	0.070	0.070
GDSS-WC-S++	**0.019**	**0.062**	**0.004**	**0.028**	**0.031**	**0.050**	**0.003**	**0.028**	**0.105**	**0.004**	**0.061**	**0.057**
HGDM-OC	0.065	0.119	0.024	0.069	0.125	0.625	0.371	0.374	0.181	0.019	0.112	0.104
HGDM-OC-S++	**0.021**	**0.034**	**0.005**	**0.020**	**0.080**	**0.500**	**0.225**	**0.268**	**0.023**	**0.034**	**0.004**	**0.020**
HGDM-WC	0.017	0.050	0.005	0.024	0.045	0.049	0.003	0.035	0.137	0.004	0.048	0.069
HGDM-WC-S++	**0.021**	**0.024**	**0.004**	**0.016**	**0.040**	**0.041**	**0.005**	**0.029**	**0.123**	**0.003**	**0.047**	**0.058**
GSDM-OC	0.142	0.230	0.043	0.138	0.930	0.867	0.168	0.655	1.996	0.0	1.013	1.003
GSDM-OC-S++	**0.011**	**0.016**	**0.001**	**0.009**	**0.012**	**0.087**	**0.011**	**0.037**	**1.2e-4**	**0.0**	**1.2e-4**	**0.066**
GSDM-WC	0.011	0.016	0.001	0.009	0.013	0.088	0.013	0.038	0.002	0.0	0	7.2e-5
GSDM-WC-S++	**0.011**	**0.016**	**0.001**	**0.009**	**0.011**	**0.086**	**0.010**	**0.036**	**5.0e-5**	**0.0**	**1.1e-5**	**0.066**