

Erratum discussion

Bai Q, Xu T, Huang J, Pérez-Sánchez H. Geometric deep learning methods and applications in 3D structure-based drug design. *Drug Discov Today*. 2024;29(7):104024.

<https://doi.org/10.1016/j.drudis.2024.104024>

Due to compatibility issues with the proof system, some formulas are not shown in the above paper, the parts that need to be modified as follows:

1) The content below Equation (28) on page 9 in the above paper (*Drug Discov Today*. 2024;29(7):104024):

$$\tilde{x}^k = \tilde{x}^{k-1} - \eta \nabla_x E_\theta(\tilde{x}^{k-1}) + \omega \quad (28)$$

Where $\omega \sim \mathcal{N}(0, \sigma)$ and $\tilde{x}^K \sim q_\theta$. The

Where $\omega \sim \mathcal{N}(0, \sigma)$ and $\tilde{x}^K \sim q_\theta$ should be **modified** to Where $\omega \sim \mathcal{N}(0, \sigma)$ and $\sigma = \delta \epsilon^\tau$. δ is the step size, $\epsilon^\tau \sim \mathcal{N}(0, I)$, and τ indexes the time.

For more details, please see reference 1.

References

1. Gao R, Song Y, Poole B, Wu YN, Kingma DP. Learning energy-based models by diffusion recovery likelihood. arXiv preprint arXiv:2012.08125. 2020. <https://arxiv.org/abs/2012.08125>