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 are as follows:

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

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

Where ω $\mathcal{N}(0,\sigma)$ and $\tilde{x}^K$ q_θ. The

"where ω $\mathcal{N}(0,\sigma)$ and $\tilde{x}^K$ q_θ." should be **modified** to "where ω is the added noise and $\omega \sim \mathcal{N}(0,\sigma)$. σ is the noise standard deviation."

For more details, please see references 1 and 2.

References

1. Gao R, Song Y, Poole B, Wu YN, Kingma DP. Learning energy-based models by diffusion recovery likelihood. arXiv preprint arXiv:201208125. 2020. https://arxiv.org/abs/2012.08125
2. Du Y, Mordatch I. Implicit Generation and Generalization in Energy-Based Models. arXiv preprint arXiv:190308689. 2020. https://doi.org/10.48550/arXiv.1903.08689