VIDY Reading Group

Jan 10 - GeoDM - Summary

Contribution:

- Propose a latent diffusion model to generate molecules with the equivariance property.

- To incorporate the equivariance, the authors propose to represent the latent representation of the molecule as the point-structured variables with which each atom has 3-d equivariant and k invariant latent features. The networks parametrize the autoencoder and denoising model in diffusion are equivariant graph neural networks.

- Modeling in latent space helps smoothen the diffusion process and reduce the generation complexity (with fewer latent features).

- The empirical results are quite impressive.

Weakness:

- L_regularization: a Kullback-Leibler regularization of qφ towards standard Gaussians is applied similarly to variational AE. However, it does not work because KL loss may distort the equivariance property. As an alternative, they use early stopping as a regularization for the encoder. A more rigorous approach should be investigated.

Longfeng's question:

- How to choose the number of steps T in the diffusion process.
  - Jialin's answer: For discrete diffusion, a few steps would be sufficient. However, for continuous diffusion, the number of steps is often a few hundred to thousands.

- Why is the Gaussian distribution chosen in the diffusion model? Are there any other alternative distributions?
  - Jialin's answer: We have a closed-form formula for the Gaussian distribution.
  - In the discrete diffusion model, we use the Bernoulli distribution.
- How does latent modeling in the proposed method contribute to controllable molecule generation?
  - Lower dimension → higher efficiency.

Jiayuan Chen's Questions

1. Potential application of the framework of Latent variable + DM to other fields.

   a. This framework can potentially work for multimodal generations. However, it should be investigated more.

2. In the Controllable Molecule Generation task on QM9, there is large discrepancy between the properties of molecules generated by the model and the standard values.

   a. Even though it has potential applications in many domains like drug discovery, the current SOTA of molecule generation is still far from practical use.

Zheng Huang's Questions

1. How the generated molecules meet chemical constraints:
   - They do not explicitly involve chemical constraints in the model except equivariance. But it might be a future direction to impose these chemical properties.
2. Time complex of the framework
   - In the image domain, they may train a GAN model to reconstruct the noise to skip some steps to speed up the denoising process.