[3L1-GS-11]AI and Society

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Thu. Jun 8, 2023 9:00 AM - 10:40 AM Room L (C2)

10:00 AM - 10:20 AM

[3L1-GS-11-04]Sample-Efficient De Novo Chemical Design with Latent Reconstruction-Aware Variational Autoencoder

○Onur Boyar[1], Kazuki Iwata[2], Hiroyuki Hanada[3], Ichiro Takeuchi[1,3] (1. Nagoya University, 2. Nagoya Institute of Technology, 3. RIKEN)

Keywords:Variational Autoencoders, De Novo Chemical Design, Bayesian Optimization

Generative models have a wide range of applications in de novo chemical design. A common choice of generative model for de novo chemical design tasks is Variational Autoencoders, which convert the high-dimensional discrete representation of chemical compounds into real-valued continuous vector representations using their encoder network. Continuous representations allow us to use optimization techniques to obtain chemical compounds with desired properties. However, due to the costly nature of evaluating the properties of the generated chemical compounds, the sample efficiency of the optimization process is crucial. The general approach is to use Bayesian Optimization in the latent space of the Variational Autoencoder model, which has many challenges yet to be tackled, such as the quality and diversity of the generated chemical compounds. In our study, we propose an approach to improve the sample efficiency of the optimization process. We propose a novel generative model, the Latent Reconstruction-Aware Variational Autoencoder, and incorporate it into the Latent Space Bayesian Optimization framework. Our results show that the proposed approach can improve the quality and diversity of the generated chemical compounds.