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Data representations for deep learning and chemistry-related applications

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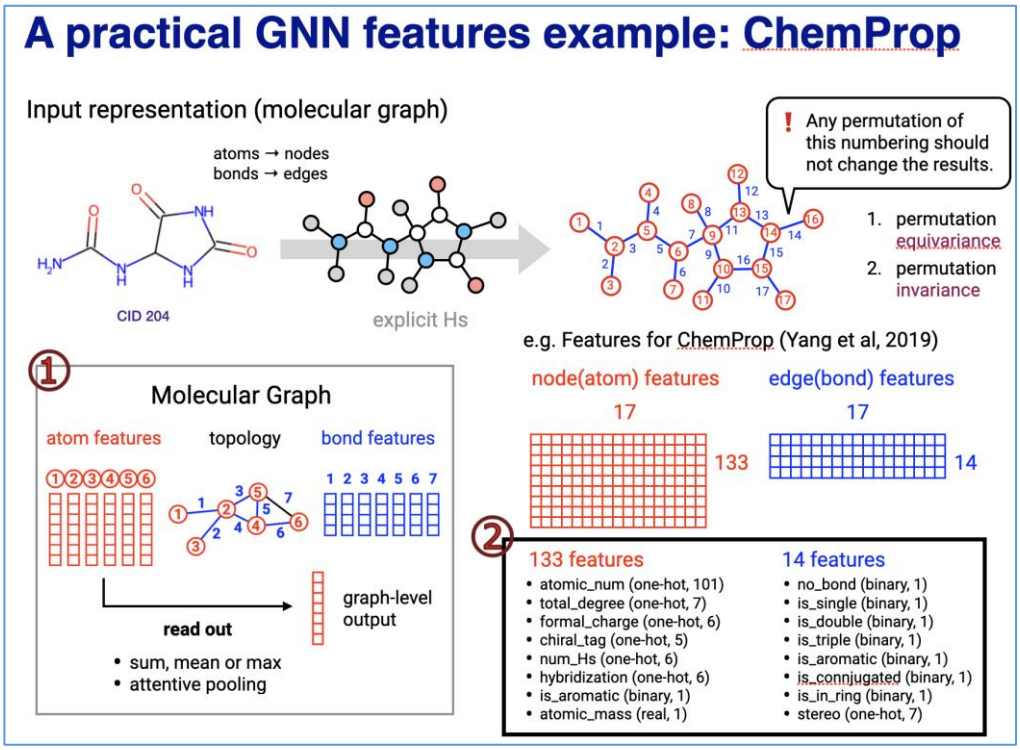
Due to surprising success of deep neural network (DNN) models these days, two categories of representations used in DNN-based models emerge in the drug discovery domain.

In this talk, we present our recent study[1] on a GNN-based molecular graph generation system, to allow users to edit the intermediate graph candidates during the molecule design process in multiple steps, utilizing the edit operation to predict the user's real intention to improve effectiveness. We design an interactive substructure-by-substructure adopt process to verify this idea. This process guarantees the involvement of user decisions to interact with a generative user-centered AI system, which differentiates our work from previous studies that generate graphs in a single run. We test our system using a real-world molecular dataset containing nearly one million graphs to show the performance. (An example of GNN features is shown in Figure below)



Reference

1. S. Hu, I. Takigawa, C. Xiao, Edit-Aware Generative Molecular Graph Autocompletion for Scaffold Input, **The 36th AAAI Conference on Artificial Intelligence (AAAI) Workshop on Deep Learning on Graphs (DLG)** (2022)

Sheng Hu. Nagoya University (ph.D. of Information Science, 2019). Kyoto University (2019~2020). ICReDD, Assistant Professor (2020~). [Field of research] Deep Learning on Graphs, Data Wrangling, Information Retrieval.