Report III : Molecular machine learning with conformer ensembles

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Overview of the Approach

A potential in silico regularly utilized in the drug development process is virtual screening. Scientists can use the program to find potential candidates for experimental investigation. The cost and time required to bring a novel drug to market can be decreased by automatically identifying promising new drug candidates. In the human body, molecules often adopt a particular three-dimensional configuration referred to as conformation. These molecules are not static. In other words, these molecules are able to rotate or spin since they are not rigid. We can define a molecular ensemble by compiling all the permitted conformational mobility. This is significant because it enables us to examine a more accurate model of the molecule in its environment.

Current approaches are used to establish three-dimensional conformations of molecules separated into two categories: physics-based simulations and, data-driven supervised models. As physics-based simulations, computational docking and molecular simulation are constrained by scoring functions and force fields, whereas machine learning methods' performance depends on the availability of data. Methods of supervised learning may be preferred because of the advantages listed below: In theory, a neural network can learn any function. Supervised prediction is a significant upgrade over physics-based techniques in terms of speed and performance. For example, neural networks can learn how to map molecules based on their physical properties.

Can three dimensional information from numerous conformers enhance molecular properties that predicted by deep learning methods is the main research question that this work seeks to answer. Multiple deep learning models have been trained to address this question by incorporating multiple conformer inputs and conformer attention to key architectures such as *ChemProp* and *Schnet*. Axelrod and Gomez-Bombarelli (2020)

Discussion

References

Axelrod, Simon, and Rafael Gomez-Bombarelli. 2020. "Molecular machine learning with conformer ensembles," December. https://doi.org/10.48550/arxiv.2012.08452.

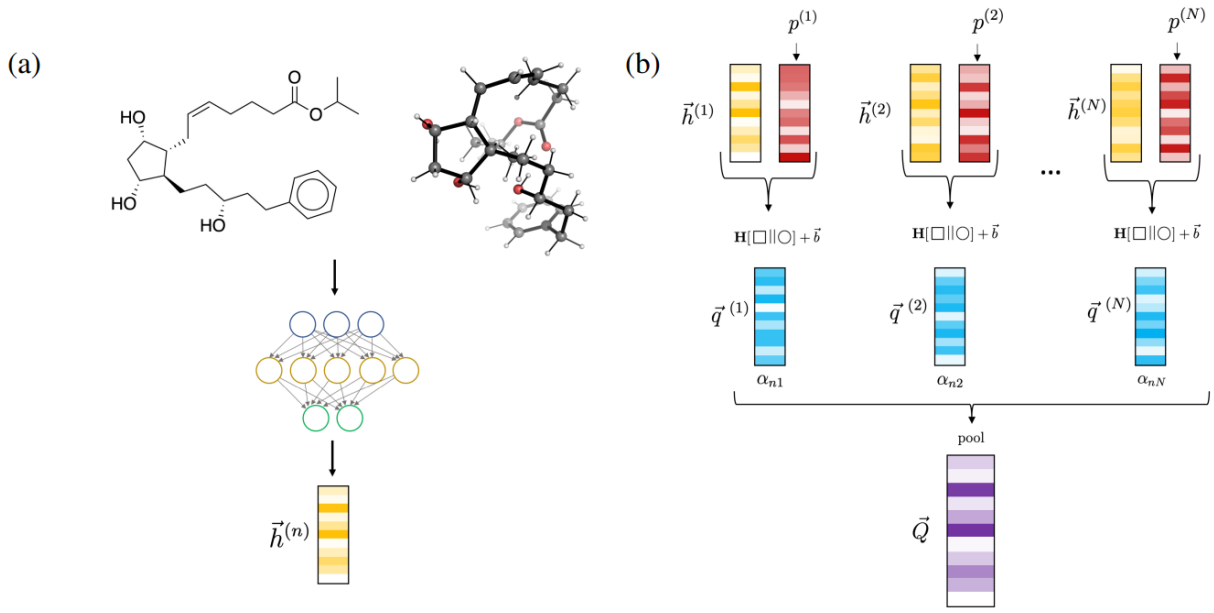

Figure 1: Overwiew of the methdology.