Simulation of Nanosystems for Energy Conversion
Department of Electrical and Computer Engineering
Technische Universität München

Deep learning-based drug discovery against Corona viruses

Motivation

Advanced deep learning techniques have the potential to bring a breakthrough in the field of drug discovery. The project aims to advance the application of deep learning in developing more accurate *in-silico* early-stage prediction of novel leads against the recently emerged corona virus SARS-COV-2. The work will directly affect both the fields of AI and Healthcare. We are currently in a situation with urgent need of expediting drug discovery process, possibly using AI. The pandemic caused by the SARS-CoV-2 virus, the disruption to daily lives, the increasing death toll and the consequential severe global economic crisis is a dire warning for us to heavily invest in healthcare systems as a preparation for such future pandemics.

Goals

1. Develop a deep learning based scoring function to enable the rapid virtual identification of lead molecules for experimental validation and optimisation: By combining two types of fingerprints of protein-ligand interactions: a) Graph Neural Network (GNN) capturing the connectivity of the interactions and b) Many Body Tensor Representation (MBTR) capturing the spatial characteristics of the interactions. Deep learning architecture will be build hybridizing these two unique types of features to construct a scoring function that has the potential to produce unprecedented accuracy in predicting the binding free energy of ligands to proteins. The scoring function will be rigorously validated against available benchmark datasets.

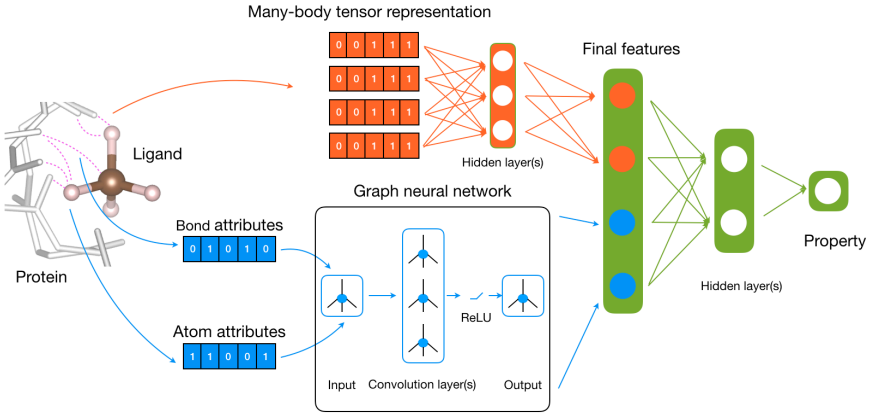
2. Generate novel inhibitor molecules: A generative model will be build based on the deep learning architecture to design novel molecules with high binding affinities to the main protease (Mpro) of the SARS-CoV-2 Corona virus. The molecules will be synthesized in collaboration with an experimental group. The experimental data would be used as a feedback to improve the accuracy of the computational model. Further medicinal chemistry on the best molecules will lead to further data to evaluate the model while progressing useful molecules against this important target.

Requirements

- Interest in drug discovery
- Experience with machine learning and deep learning
- Programming knowledge

Duration

This topic is suitable for Masters thesis (6-12 month).



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1. **Rahaman O.**, Estrada T. P., Doren D. J., Taufer M., Brooks C. L., III and Armen R.S., *J. Chem. Inf. Model., 51 (9), 2047-2065* (2011)