For favour of Posting

THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

Department of Mathematics

PhD Student Seminar

Surface Distance Aided Geometric Deep Learning for Binding Conformations

By

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Abstract

A core task in computer-aided drug discovery is the optimization of lead compounds with high binding affinity to the target proteins. The binding process is desired to find the proper position and the correct relative orientation of the ``key'' (the ligand), which will open up the ``lock'' (the protein). During the process, existing deep learning methods usually overlook surface intersection between ligands and targets, i.e., part of the ligands goes into the protein interior. In this paper we present our SurfBind model, a two-stage deep learning method aided by the surface distance function (SDF). SurfBind will produce pairwise distance distribution to encode the multi-valued possible relative positions. By exerting effective SDF constraint to distance likelihood potential, SurfBind derives rational conformations lessening clash to the protein, and also reduces root mean square deviation (RMSD) for ultra-large ligands. Compared to Deepdock, Surfbind increases the top1 docking power by 8.8% and the forward screening power by 10.5% on CASF-2016 benchmark.

Date : 4 May 2023 (Thursday)
Time : 11:00 am
Venue : Room 5501 (Lifts 25/26)

All are Welcome!