BRIGHAM AND WOMEN'S HOSPITAL
HARVARD MEDICAL SCHOOL

181 Longwood Avenue
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Department of Medicine
Channing Division of Network Medicine

Channing Methods Seminar

December 6, 2022, 11AM (ET)

MCP 5th-floor large conference room
https://us02web.zoom.us/j/579497999?pwd=cHNlWHMzWUlFUUVJTG1EeVJmY05aQT09
Meeting ID: 579 497 999
Passcode: 844168

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Identifying interactions between novel protein targets and ligands - AI-Bind and AI-assisted molecular docking

Identifying potential drug-target interactions (DTI) is a critical step in accelerating drug discovery. Although numerous machine learning models have significantly expedited the drug development process, these models leverage the topology of the DTI network (training data) and fail to generalize to novel proteins and ligands. We will discuss how these models exploit topological shortcuts, and how AI-Bind combines network science and unsupervised pre-training in improving the generalizability of the binding prediction task. Beyond making accurate binding predictions for never-before-seen molecular structures, AI-Bind can identify potential binding locations on the proteins even with limited data. Lastly, the integration of AI-bind with AutoDock Vina improves the process of molecular docking compared to a blind approach.

Short bio: Ayan Chatterjee is a fourth-year Ph.D. student under the supervision of Prof. Tina Eliassi-Rad at the Network Science Institute, Northeastern University, Boston. Ayan is interested in graph machine learning, specifically link prediction, graph embeddings, the expressivity of GNNs, and XAI. Prior to joining NetSI, he worked at NVIDIA Graphics, developing and optimizing GPU architectures for AI applications and gaming.