



# BIOINFORMATICS SEMINAR

## YASAMAN MOGHADAMNIA

*Graduate Student, UNIVERSITY OF DELAWARE*

### MATHEMATICAL MODELING OF ARVS DIFFUSION INTO THE LYMPH NODES TO INVESTIGATE DRUG TRANSPORT MECHANISMS

Direct imaging of anti-retroviral (ARV) distribution in rhesus macaque (RM) lymph nodes (LNs) show concentration variations of 10-30-fold within the same LN. Barriers between the blood, sinus, and lobule may hinder free drug transport; therefore, cell-mediated ARV transport may dominate despite being much slower. We evaluate this hypothesis using a predictive model of drug distribution within a lymph node lobule. This model solves PK reaction and spatial diffusion dynamics on a fully reconstructed 3D geometry of a murine LN, reproducing observed spatial pattern of ARV distribution. To construct the 3D model high resolution confocal imaging, segmentation, and volumetric anatomical reconstruction were used. The spatially created patterns show agreement with experimentally observed patterns. Therefore, this model provides a valuable tool for designing better and more effective antiretroviral and anticancer drugs.

#### BIOGRAPHY

Yasmin was born in Iran. She completed her college and first master's degree in Alzahra University, Tehran, Iran, both in physics. She worked on modeling cancerous tumor growth and the effects of environmental disturbances on the tumor cell number. She received her second master's degree in molecular biophysics at Johns Hopkins University. Her work at Hopkins included stochastic modeling of protein-protein interactions and usage of techniques such as molecular dynamics to understand biological systems on a molecular level. She is now a second-year PhD student in the Bioinformatics and Data science program. Her two PIs, Dr. Ryan Zurakowski and Dr. Jason Gleghorn are professors in the Biomedical engineering department at UD. Her current work includes modeling of sanctuary site behavior in treating HIV and 3D reconstruction of full-tissue geometry of mouse lymph nodes.

## XIHAN QIN

*Graduate Student, UNIVERSITY OF DELAWARE*

### GRAPH ENCODER EMBEDDING AND GRAPH SEMI-SUPERVISED LEARNING

Graphs are widely used in many research areas. Graph analytics is essential to gaining information from graphs. To learn from the graphs, graph embedding is needed to capture the key features and provide a fixed-sized matrix for machine learning methods. However, the current graph embedding suffers the high computation and space costs. There is room to improve the accuracy. I will introduce our new graph embedding method called Graph Encoder Embedding (GEE) and show how using GEE for machine learning methods, Linear discriminant analysis (LDA) and Neural Networks (NN), has significantly better performance than Node2Vec. The test datasets include simulated graphs from Stochastic Block Model (SBM) and Degree-Corrected Stochastic Block Model (DC-SBM), and benchmark datasets from Network Depository. I will show how we adopt GEE for a new semi-supervised learning method and its outstanding testing results on simulated data and touch upon the exciting future work including more evaluations of our current methods and an exploration of using GEE for different graph learning tasks.

#### BIOGRAPHY

Xihan Qin is a PhD student in Computer Science. She works in Dr. Shen's lab in the Department of Applied Economics and Statistics. Dr. Liao from the department of Computer and Information Sciences is her co-advisor. She has a MS degree in Bioinformatics from UD. Her current research is on Graph embedding and Graph machine learning. She is looking forward to applying those new methods to biological graph analysis

**CBCB SEMINAR**

**5/16/2022**

**3:30-4:30PM**

**AP BioPharma**

**Room 140**

**(590 Avenue 1743)**

**or via ZOOM:**

**[https://udel.zoom.us/j/](https://udel.zoom.us/j/93068494454)**

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**[bioinformatics.udel.edu](http://bioinformatics.udel.edu)**

