ELECTRICAL & COMPUTER ENGINEERING BIO-SEMINAR Fall 2020 TEXAS A&M UNIVERSITY Engineering

When: **Friday 16:15 – 17:05, August 28, 2020**
Where: https://tamu.zoom.us/j/514754727

Speaker: **Mostafa Karimi**

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Title: **Network-Principled Deep Generative Models for Designing Drug Combinations as Graph Sets**

Abstract: Combination therapy has shown to improve therapeutic efficacy while reducing side effects. Importantly, it has become an indispensable strategy to overcome resistance in antibiotics, antimicrobials and anticancer drugs. Facing enormous chemical space and unclear design principles for small-molecule combinations, computational drug-combination design has not seen generative models to meet its potential to accelerate resistance-overcoming drug combination discovery. We have developed the first deep generative model for drug combination design, by jointly embedding graph-structured domain knowledge (gene-gene, gene-disease, and disease-disease) and iteratively training a reinforcement learning-based chemical graph-set designer. Numerical results indicate that, compared to state-of-the-art graph embedding methods, hierarchical variational graph auto-encoder learns more informative and generalizable disease representations. Results also show that the deep generative models generate drug combinations following the principle across diseases with low toxicity. The generated drug combinations collectively cover the disease module similar to FDA-approved drug combinations and could potentially suggest novel systems pharmacology strategies. (This is a joint work with Arman Hassanzadeh)

Bio: Mostafa Karimi is a PhD student of Electrical and Computer Engineering at Texas A&M University under supervision of Dr. Yang Shen. Prior to that, he received double bachelor degrees in Electrical Engineering and computer science from Sharif University of Technology in 2015. His research focuses on combinatorial optimization, protein modeling, and deep learning.