



Talk information

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Title of the talk:

GeNNius: An ultrafast drug-target interaction inference method based on graph neural networks

Abstract of the talk:

Drug-target interaction (DTI) prediction is a relevant but challenging task in the drug repurposing field. In-silico approaches have drawn particular attention as they can reduce associated costs and time commitment of traditional methodologies. Yet, current state-of-the-art methods present several limitations: existing DTI prediction approaches are computationally expensive, thereby hindering the ability to use large networks and exploit available datasets and, the generalization to unseen datasets of DTI prediction methods remains unexplored, which could potentially improve the development processes of DTI inferring approaches in terms of accuracy and robustness.

In this work, we introduce GeNNius (Graph Embedding Neural Network Interaction Uncovering System), a Graph Neural Network (GNN)-based method that outperforms state-of-the-art models in terms of both accuracy and time efficiency across a variety of datasets. We also demonstrated its prediction power to uncover new interactions by evaluating not previously known DTIs for each dataset. We further assessed the generalization capability of GeNNius by training and testing it on different datasets, showing that this framework can potentially improve the DTI prediction task by training on large datasets and testing on smaller ones. Finally, we investigated qualitatively the embeddings generated by GeNNius, revealing that the GNN encoder maintains biological information after the graph convolutions while diffusing this information through nodes, eventually distinguishing protein families in the node embedding space.

Biography of the speaker:

Dr. Ochoa graduated with B.Sc. and M.Sc. degrees in Telecommunication Engineering (Electrical Engineering) from the University of Navarra (Tecnun), Spain, in 2009. She then obtained a MS and a PhD in the Electrical Engineering Department at Stanford University in 2012 and 2016, respectively. Dr. Ochoa has performed internships as a software engineering at Google, CA and Genapsys, CA. She also served as a technical consultant for the HBO show “Silicon Valley”. After obtaining the PhD, Dr. Ochoa joined the faculty at the Electrical and Computing Engineering department at the University of Illinois at Urbana-Champaign (UIUC), as an assistant professor. She then joined the faculty at Tecnun as a collaborator professor in January 2020.

Her research interests include computational biology, data compression, bioinformatics, information theory and coding, machine learning, communications, and signal processing. Her research focuses on the development of computational methods tailored to omics data, to aid the storage, handling, and analysis of



these data. She has developed several compression algorithms for genomic, methylation and mass spectrometry data that are currently the state-of-the-art, some of which are now part of the standard MPEG-G for the representation of genomic information being developed under ISO (International Standardization Organization).

Dr. Ochoa's graduate studies were funded by a Stanford Graduate Fellowship and a La Caixa Graduate Fellowship. She has been awarded the MIT Innovators under 35 award (2019), the Gipuzkoa Fellows (2020), and a Ramon y Cajal grant (2020), for the importance of her potential and innovative research.

