

Speaker: Marinka Zitnik, Harvard

*Title:*

Learning actionable representations of biomedical data

*Abstract:*

The success of machine learning is heavily dependent on the choice of data features on which the methods are applied. For that reason, much of the actual efforts in deploying algorithms go into engineering of features that support effective machine learning. In this talk, I describe our efforts to expand the scope and ease the applicability of machine learning on rich graph datasets and knowledge networks. First, I outline our methods for graph representation learning. The methods specify deep graph neural functions that map nodes in a graph to points in a compact vector space, termed embeddings. These graph neural methods are optimized to embed graphs such that performing algebraic operations in learned embedding spaces reflects the topology of input graphs. We show how embeddings enable repurposing of drugs for new indications and discovery of dozens of drug combinations that are safe in patients with considerably fewer unwanted side effects than today's treatments. Further, embeddings allow for accurate molecular phenotyping by identifying drug targets, disease proteins, and molecular functions better than much more complex algorithms. Lastly, I describe our efforts in learning actionable representations that allow users of our models to ask what-if questions and receive predictions that are accurate and can be interpreted meaningfully.