

Learning the Dynamics of Biological Networks with Deep Graph Networks

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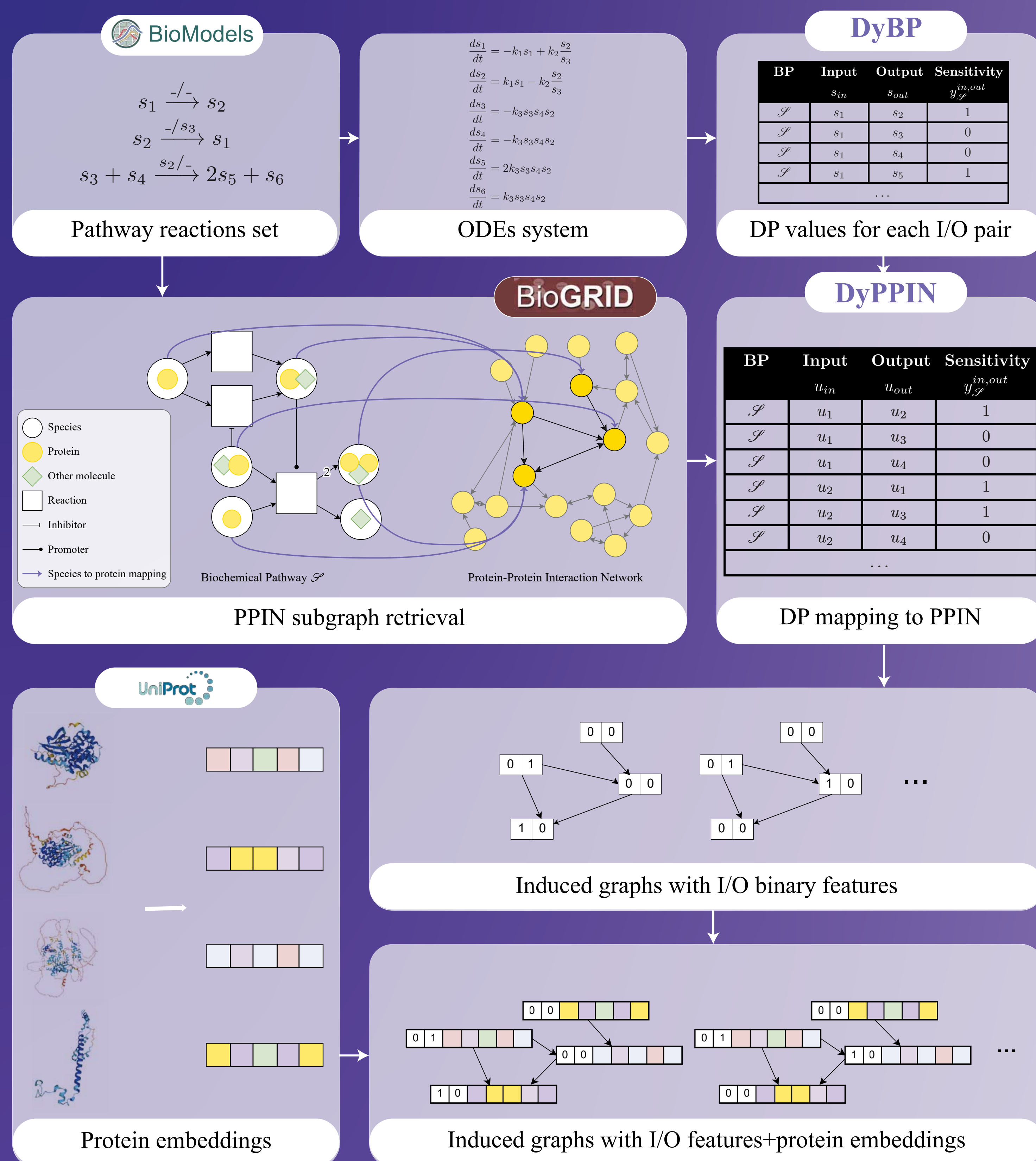
Problem Biological systems can be described by complex networks. As this graph data grows in size, modeling the dynamics of the underlying dynamical system in terms of chemical reactions becomes a tougher challenge. High level networks, like Protein-Protein interaction Networks (PPIN), are described and analyzed as static objects, but the systems biology community calls for methods that are able to model them taking into account their dynamical nature.

Can we learn a model to study dynamics of large scale networks?

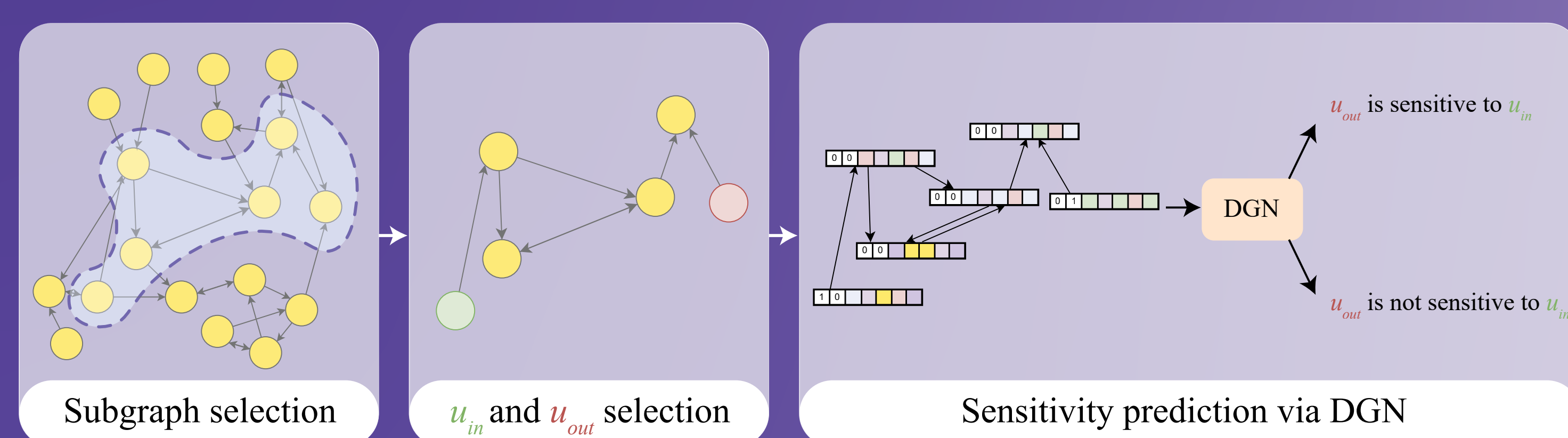
Proposed solution We designed a pipeline that enables the prediction of sensitivity over Protein-Protein Interaction Networks.

What's next?

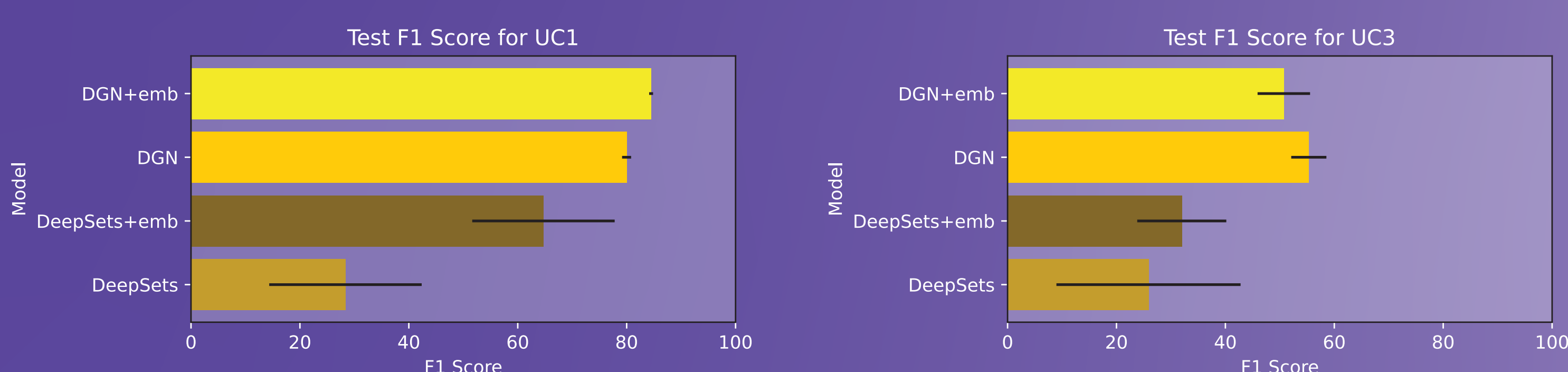
Dataset Extraction



Dynamical property prediction



Results The PPIN structure allows to predict the sensitivities derived from biochemical pathways with high accuracy.



Computational Biology applications

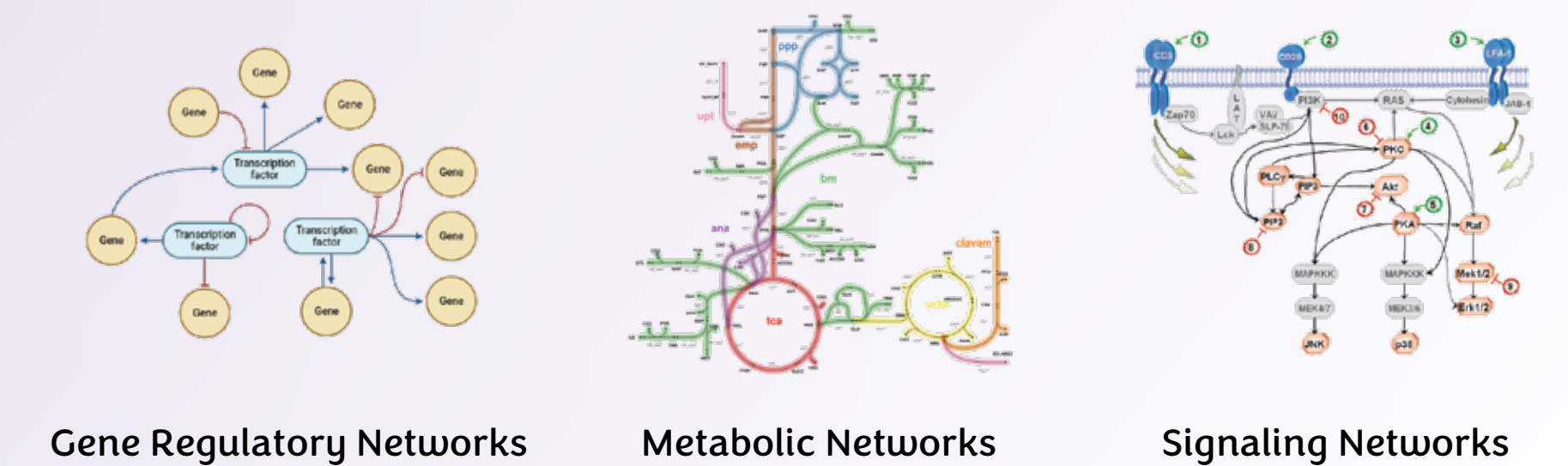
Dynamics modeling and prediction over whole interactome



Embed information from non-simulable pathways



Extension to more biological networks

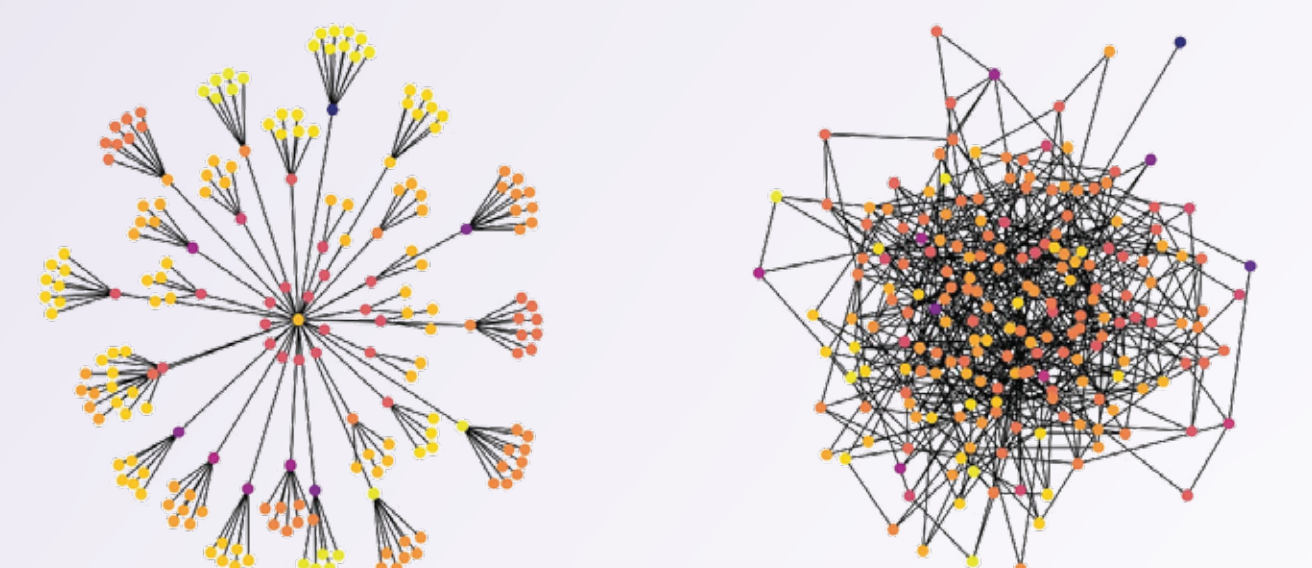


Case studies

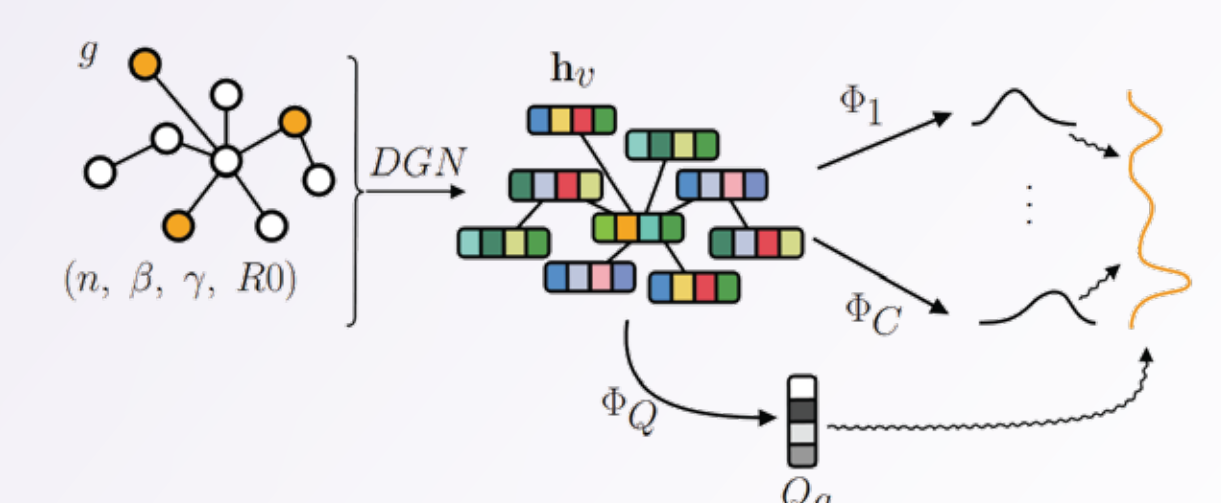


Research on Deep Graph Networks

Deal with heterophily and long range dependencies within large and dense networks



Probabilistic models to estimate multiple dynamics



Reservoir computing models to approximate cellular dynamics

