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Description

Technological advances in experimental biology provide us with an astounding amount of various molecular and clinical data describing different aspects of the functioning of the cells. These complex big data carry biomedical information that is currently hidden from us within their large sizes and complexities. Hence, some of the foremost computational challenges that the data pose are:

- 1) how to analyse complex omics networks individually;
- 2) how to analyse them jointly; and
- 3) how to comparatively extract new biomedical information.

These challenges are not trivial and require the development of heuristic new algorithms due to the computational intractability of the underlying problems. This project addresses several such algorithmic challenges that the data pose and applies the new algorithms to the most up-to-date, versatile omics data. In a cell, molecules interact in pair wise fashion, but also jointly to form larger molecular machines. Hence, omics data are naturally represented both by simple graphs, as well as by models that capture multi-scale molecular organization, including hypergraphs and abstract simplicial complexes.

Prof. Przulj introduced graphlets as a sensitive algorithmic tool that measures the structure (topology) of networks and nodes. They have since become a highly-cited, important tool for algorithmic development yielding substantial domain specific insight in many areas, including biology. Prof. Przulj generalised graphlets to hypergraphlets and simplets to enable analyses of multi-scale models of molecular interactions modelled by hypergraphs and abstract simplicial complexes.

However, none of these allow for weights on edges, while molecular networks are naturally weighted. For this reason, the project proposes extensions of algorithms that use graphlets, hypergraphlets and simplets to compute with weights on edges and thus include this important biological information into mining algorithms. The project also generalises Graphlet Laplacians to deal with automorphism orbits of graphlets, as well as graphlet based clustering coefficients uniting graphlet and clustering properties of networks.

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