Optimization-based computation of biochemical reaction network structures

Kinetic systems form a general class of nonlinear dynamical models that is suitable to describe complex nonlinear phenomena not only in (bio)chemical processes but in other fields as well, where the state variables are constrained to be nonnegative [1]. A dynamical model given in the form of ODEs is kinetic if a weighted directed graph (i.e., a chemical reaction network) can be assigned to it, which realizes the dynamics. Necessary and sufficient conditions for the kinetic property of a polynomial ODE were given in [2] and it is known that the reaction graph corresponding to a given dynamics is non-unique. However, in chemical reaction network theory, strong results have been developed on the relations between network structure and the dynamical properties (stability, existence/uniqueness of equilibria, boundedness of solutions etc.) of the system. Therefore, it is of interest to study whether there exist such network structures/parametrizations for a set of kinetic ODEs that guarantee a desired property. In this lecture, a summary of computational methods mostly based on linear programming will be presented that can be used to study the existence and compute reaction graphs with preferred properties such as minimal/zero deficiency, complex/detailed balance or weak reversibility [3-6].