

Analysis of Biochemical Reaction Networks using Tropical Geometry and Pathway-Based Methods

Abstract:

The core idea of computational systems biology is to view biological systems as complex non-linear dynamical networks of molecular parts. These networks have emergent collective behaviors that are explainable only if the constituting parts of the system and their mutual interactions are considered. Most often, such systems are modelled using Ordinary Differential Equations (ODEs).

For large networks with ODE based dynamics and multiple timescales it is reasonable to consider that a typical trajectory consists of a succession of qualitatively different slow segments separated by faster transitions. The slow segments, generally are called as Metastable Regimes (MRs). In this talk, it will be explained how the solutions based on tropical geometry can be used as proxies for such MRs. The application of such an approach in cancer biology will be discussed. In addition, it will also be demonstrated how the tropical solutions can be used for computing a simpler description of the system by timescale separation, popularly known as model reduction. Ultimately, this can help to determine the key variables and processes of the system.

For systems, whose ODE dynamics is unknown (due to uncertain parameters or rate laws) but the underlying biochemical reaction network structure is known, the applicability of pathway-based methods namely extreme currents will be shown. Such pathways will be used as network features in the context of statistical learning to discriminate between clinical phenotypes (e.g. healthy vs disease , censored survival times).

Finally, preliminary ideas to integrate mechanistic and data driven approaches in the context of systems biology will be presented.