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Large deviations theory for chemical reaction networks

At the microscopic level, the dynamics of arbitrary networks of chemical reactions can be modeled as jump Markov processes whose sample paths converge, in the limit of large number of molecules, to the solutions of a set of algebraic ordinary differential equations. Fluctuations around these asymptotic trajectories and the corresponding phase transitions can in principle be studied through large deviations theory in path space, also called Wentzell-Freidlin (W-F) theory. However, the specific form of the jump rates for this family of processes does not satisfy the standard regularity assumptions imposed by such theory, and weaker conditions need to be developed to deal with the framework at hand.

Using tools of Lyapunov stability theory we design sufficient conditions for the applicability of large deviations estimates to the asymptotics of the Markov process at hand. We then translate such conditions in terms of the topological structure of the chemical reaction network. This ultimately allows to define a large class of chemical reaction systems to which the estimates of interest can automatically be applied.