Symbolic bifurcation analysis of reaction networks with Python. Part I: Theory

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Computer algebra methods for analyzing reaction networks often rely on the assumption of mass-action kinetics, which transform the governing ODEs into polynomial systems amenable to techniques such as Gröbner basis computation and related algebraic tools. However, these methods face significant computational complexity, limiting their applicability to relatively small networks involving only a handful of species.

In contrast, building on recent theoretical advances, we present a symbolic approach designed to detect bifurcations in larger reaction networks (up to a few dozen species) equipped with a broad class of "parameter-rich" kinetics. This class includes enzymatic kinetics such as Michaelis-Menten, ligand-binding kinetics like Hill functions, and generalized mass-action kinetics.

For a given network, the algorithm identifies all minimal autocatalytic subnetworks and fully characterizes the presence of bifurcations associated with zero eigenvalues, thus determining whether the network admits multistationarity. It also effectively detects oscillatory bifurcations arising from positive-feedback structures, capturing a significant class of possible oscillations.

The first talk (Vassena) will cover the theoretical foundations of this method, while the second (Golnik) will address its implementation in Python.