SC-Square Methods for the Detection of Hopf Bifurcations in Chemical Reaction Networks

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To fit the SIAM AG programme this talk is in two parts: the first is introductory, the second more detailed.

Abstract

First part: background and and basic methods

The analytical problem of finding Hopf bifurcation fixed points for polynomial or rational vector fields (or determining that there are none) can be reduced to a purely semi-algebraic question. In the first part of the talk we explore this possibility by first giving a reduction of the parametric question on the existence of a Hopf bifurcation fixed point to a parametric first-order formula over the ordered fields of the real. We show the results of solving these with existing tools from computational logic (such as *Redlog*) for several standard and text book examples and compare the results of these fully automated methods to the ones of hand analyses given in textbooks.

Second part: advanced methods for chemical reaction networks

The determination of Hopf bifurcation fixed points in chemical reaction networks with symbolic rate constants yields information about the oscillatory behavior of the networks and hence is of high interest. The problem is solvable in theory by the methods discussed in the first part, but the generic technique leads to prohibitively large formulæeven for rather small dimensions. Using the representations of chemical reaction systems in convex coordinates, which arise from the so called stoichiometric network analysis, the problem of determining the existence of Hopf bifurcation fixed points leads to first-order formulæover the ordered field of the reals that can then be solved using existing computational logic packages for somewhat larger dimensions. Using ideas from tropical geometry it is possible to formulate a more efficient method that is incomplete in theory but works very well for the examples that we have attempted; we have shown it to be able to handle systems involving more than 20 species. Finding satisfying instances of a single (but in general very large) polynomial equation and a set of polynomial inequalities is the key challenge, which will benefit from further research in the context of SC-square-methods.

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