Using ML tools to predict number of solutions of parametric system of polynomial equations with the help of CRNs

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Many questions in Chemical Reaction Network (CRN) theory can be framed as classifica- tion problems, such as the detection of multistationarity. In the age of AI, it is a common knowledge that there are plenty of machine learning (ML) algorithms capable of doing classi- fication tasks. These two sentences just made a clear motivation for using ML tools in CRN theory, and recently, in a work by the speaker and his colleagues, the first step in this direction has been taken. They introduced a new representation for CRN objects that helps us feed a CRN as an input to advanced ML algorithms. Multistationarity of a network mathemati- cally is the study of number of (positive) real solutions to a parametric system of polynomial equations describing the steady states of the network. This success together with Hungarian Lemma that states any given parametric polynomial system satisfying a technical condition can be associated to steady states of a CRN, triggers yet another idea. It is known that the deterministic symbolic algorithms to study the number of real solutions of parametric system of polynomial equations such as cylindrical algebraic decomposition are doubly exponential and so not practical for large size systems. Thus, we propose to use a new approach, convert- ing the system of equations to a CRN and then using the newly developed ML tools to predict the number of real solutions of the system.

References

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