Graph-Theoretic Algorithms for Reducing Chemical Reaction Networks

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Chemical reaction networks (CRNs) serve as models for complex biochemical processes occurring in cells and tissues. Studying these models is essential for understanding diseases, developing new therapies, controlling bioengineering processes, and gaining insights into fundamental aspects of living systems. However, many existing CRN models involve a large number of species and reactions, placing them beyond the reach of formal analysis methods. Additionally, parameter optimization for such models suffers from the curse of dimensionality. In previous work, we developed model reduction techniques that transform complex CRNs into simpler ones, with fewer species and reactions, making them more amenable to analysis and optimization. These approaches were based on tropical scaling and geometric singular perturbation theory. More recently, we introduced a graph-theoretical model reduction method based on the graph Laplacian. This method transforms CRNs algorithmically using graph rewriting on the species-reaction graph. In this presentation, I will show how model reduction via singular perturbations can also be formulated as a graph rewriting process and describe a general implementation of such algorithms. I will also discuss the application of these tools for generating hierarchies of models, where each model is derived from a more complex one through reduction. Such hierarchies can be used in AutoML strategies to select an appropriate model based on the available data and to use optimization results from simpler models to constrain and inform the optimization of more complex models as richer datasets become available.