Abstract:

Understanding the algorithmic behaviors that are in principle realizable in a chemical system is necessary for a rigorous understanding of the design principles of biological regulatory networks. Coupled chemical interactions in a well-mixed solution are commonly formalized as chemical reaction networks (CRNs). However, despite the widespread use of CRNs in the natural sciences, the range of computational behaviors exhibited by CRNs is not well understood. Here we study the following problem: what functions f : Rk $\rightarrow$ R can be computed by a CRN, in which the CRN eventually produces the correct amount of the "output" molecule, no matter the rate at which reactions proceed? We prove that a function is rate-independently computable if and only if it is piecewise linear (with rational coefficients) and continuous (dual-rail representation), or non-negative with discontinuities occurring only when some inputs switch from zero to positive (direct representation).