Defining Autocatalysis in Chemical Reaction Networks

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ABSTRACT Autocatalysis is a deceptively simple concept, referring to the situation that a chemical species X catalyzes its own formation. From the perspective of chemical kinetics, autocatalysts show a regime of super-linear growth. Given a chemical reaction network, however, it is not at all straightforward to identify species that are autocatalytic in the sense that there is a sub-network that takes X as input and produces more than one copy of X as output. The difficulty arises from the need to distinguish autocatalysis e.g. from the superposition of a cycle that consumes and produces equal amounts of X and a pathway that produces X. To deal with this issue, a number of competing notions, such as exclusive autocatalysis and autocatalytic cycles, have been introduced. A closer inspection of concepts and their usage by different authors shows, however, that subtle differences in the definitions often makes conceptually matching ideas difficult to bring together formally. In this contribution we make some of the available approaches comparable by translating them into a common formal framework that uses integer hyperflows as a basis to study autocatalysis in large chemical reaction networks. As an application we investigate the prevalence of autocatalysis in metabolic networks.

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