Designing Machine Learning Tools to Characterize Multistationarity of Fully Open Reaction Networks

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Chemical Reaction Networks (CRNs) are the mathematical formulation of how the quantities associated to a set of species (molecules, proteins, cells, or animals) vary as time passes with respect to their interactions with each other. Their mathematics does not describe just chemical reactions but many other areas of the life sciences such as ecology, epidemiology, and population dynamics. We say a CRN is at a steady state when the concentration (or number) of species do not vary anymore. Some CRNs do not attain a steady state while some others may have more than one possible steady state. The CRNs in the later group are called multistationary. Multistationarity is an important property, e.g. switch-like behaviour in cells needs multistationarity to occur. Existing algorithms to detect whether a CRN is multistationary or not are either extremely expensive or restricted in the type of CRNs they can be used on, motivating a new machine learning approach. This talk is about a recent attempt to design machine learning tools to predict multistationarity of reaction networks.

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