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Identification of dynamical models of chemical reaction networks[1]

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Current first-principles models of complex chemistry, such as combustion reaction networks, often give inaccurate predictions of the time variation of chemical species. Moreover, the high complexity and dimensionality of these models render them impractical for real-time prediction and control of chemical network processes. These limitations have motivated us to search for an alternative paradigm that is able to both identify the correct model from the observed dynamical data and reduce complexity while preserving the underlying network structure. In this talk, I will present one such modeling paradigm under the scenarios of complete and incomplete observability of the dynamics. The proposed approach is applicable to combustion chemistry and a range of other chemical reaction networks.

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