DERIVATION OF STATIONARY DISTRIBUTIONS OF BIOCHEMICAL REACTION NETWORKS VIA STRUCTURE TRANSFORMATION

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ABSTRACT

Long-term behaviors of biochemical reaction networks are described by steady states in deterministic models, and stationary distributions in stochastic models. Unlike deterministic steady states, stationary distributions capturing inherent fluctuations of reactions are extremely difficult to derive analytically due to the curse of dimensionality. In this presentation, we introduce a newly developed method to derive stationary distributions from deterministic steady states by transforming reaction networks to have a special dynamic property based on chemical reaction network theory. Specifically, we merge nodes and edges to make a steady state complex balanced, i.e., the in- and out-flows of each node are equal, and then we derive a stationary distribution from the complex balanced steady state. Applying our approach to various networks, we identify robustness, sensitivity, and multi-modality of their stationary distributions. Importantly, we provide a user-friendly computational package, called CASTANET, that transforms BRNs and then analytically derives their stationary distributions.