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Weakly reversible realizations of Biochemical Systems Theory (BST) models

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Biochemical Systems Theory (BST) is a modeling framework that uses power law formulations so that nature's nonlinearities and heterogeneity can be well taken into account. It has been recently found out that reaction networks can represent BST models. However, many results in Chemical Reaction Network Theory (CRNT) require that the reaction network be weakly reversible which is usually not the case for BST models. Hence, this paper aims to obtain an algorithm to construct a weakly reversible realization of two variants of BST models which are S-systems and General Mass Action (GMA) systems.

The algorithms are based on the notion that fixing the stoichiometric matrix of the initial network preserves the dynamics of the system. For S-systems, it was done via association of reactions for the influx and efflux terms of the model such that the same set of reaction vectors are generated with the initial reaction network representation. On the other hand, GMA systems made use of matrix factorization via solving a linear system. However, the algorithm becomes impractical for large GMA systems which is then remedied by considering poly-PL kinetics and applying the algorithm for S-systems.

This paper enables us to analyze BST models using results on CRNT such as on the non-emptiness of the system's set of positive steady states. Furthermore, it enriches the field of CRNT because the proposed methods here allow us to construct a weakly reversible reaction network with power law formulations.

Keywords: chemical reaction networks, weak reversibility, biochemical systems theory, power law kinetics, poly-PL kinetics

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