

Substrate modification networks are ubiquitous in living, biochemical systems. We use a directed hypergraph, a generalization of a directed graph where a directed edge connects a nonempty set of nodes to another nonempty set of nodes, to model the substrate modifications. This substrate “skeleton” portrays information about changes to the substrates while not showing the detailed reaction steps, the identity of enzymes or that of substrate-enzyme compounds. One skeleton can underlie multiple different detailed models and reaction mechanisms. We show that certain dynamical properties, such as the existence of positive steady states or presence of concentration robustness can be inferred directly from the substrate skeleton. Concentration robustness is the property where the concentration of one species or a positive-integer linear combination of species is invariant across all positive steady states. We introduce the notion of “current” on a directed hypergraph, which is one of the two crucial ingredients along with bifunctional enzyme action required to produce concentration robustness. This approach is a departure from previous deficiency based results as it applies to arbitrary substrate modification networks. This is joint work with Tung Nguyen.