Structure and Dynamics of Complex Systems: from social media mining to control of biochemical networks

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The structure of networks has provided many insights into the organization of complex systems. The success of this approach is its ability to capture the organization of multivariate interactions, and how it changes in time (network evolution) without explicit dynamical rules for node variables. As the field matures, however, there is a need to move from understanding to controlling complex systems. This is particularly true in systems biology and medicine, where increasingly accurate models of biochemical regulation have been produced. More than understanding the organization of biochemical regulation, we need to derive control strategies that allow us, for instance, to move a mutant cell to a wild-type state, or revert a mature cell to a pluripotent state. Here I present two concepts developed in our group aimed at supporting this goal. First I will present the concept distance backbone, the invariant subgraph of the distance closure of weighted graphs [Simas and Rocha, 2015]. This backbone allows us to identify redundant edges in the computation of shortest paths; we show that there is massive redundancy in many networks in different domains, including social media, Wikipedia, functional and structural brain networks, citation, air traffic, etc [Simas et al, 2016]. Since shortest-paths and diffusion distances play a role in information dynamics unfolding on brain networks [Kolchinsky et al, 2014] and knowledge networks [Ciampaglia et al, 2015], removing redundant edges can facilitate computation and discovery of important pathways in many applications. Secondly, I will present the schema redescription methodology, used to remove redundancy from automata rules to reveal their canalization properties, thus simplifying the characterization of control in large models of natural networks, such as systems biology models of biochemical regulation [Marques-Pita and Rocha, 2013]. We demonstrate that canalization (measured as effective connectivity) is an order parameter of Boolean Network (BN) dynamics, and a major factor in network controllability [Gates and Rocha, 2016; Marques-Pita, Manicka and Rocha, 2016].