Dynamics of complex biological systems determined from minimal subsets of molecules in regulatory networks

Modern biology provides series of large networks describing regulations between many species of molecules. It is widely believed that dynamics of molecular activities based on such regulatory networks are the origin of biological functions. However, we currently have a limited understanding of the relationship between structure of a regulatory network and its dynamics. In this study we develop a general theory to provide an important aspect of dynamics from information of regulatory linkages alone. It shows that "Feedback Vertex Set" of a regulatory network is "Determining Set" of the dynamics of molecular activities. The theory is practically powerful to study biological systems. First, it assures that i) any dynamical behaviors of whole system, steady states, periodic oscillations or quasi-periodic oscillations can be identified by measurements of a subset of molecules in the network, and that ii) the subset is determined from the regulatory linkage alone. For example, all of the dynamical attractors possibly generated by a signal transduction network with 113 molecules can be identified by measurement of activity of 5 molecules, if the information of network is correct. Second, our theory provides rational criterion to select key molecules to control a system. We demonstrate the aspect using a model for mammalian circadian rhythms with 6 informative variables among 21 variables in the system. We show that controlling the dynamics of informative molecules is sufficient to switch dynamics of whole system from an attractor to others distinct from original. We will show other examples of analysis for complex biological systems.