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In silico evolution of oscillatory dynamics in biochemical networks

MD ZULFIKAR ALI, Clark University, NED S. WINGREEN, Princeton University, RANJAN MUKHOPADHYAY, Clark University — We are studying in silico evolution of complex, oscillatory network dynamics within the framework of a minimal mutational model of protein-protein interactions. In our model we consider two different types of proteins, kinase (activator) and phosphatase(inhibitor). In our model. each protein can either be phosphorylated(active) or unphospphorylated (inactive), represented by binary strings. Active proteins can modify their target based on the Michaelis-Menten kinetics of chemical equation. Reaction rate constants are directly related to sequence dependent protein-protein interaction energies. This model can be stuided for non-trivial behavior e.g. oscillations, chaos, multiple stable states. We focus here on biochemical oscillators; some questions we will address within our framework include how the oscillatory dynamics depends on number of protein species, connectivity of the network, whether evolution can readily converge on a stable oscillator if we start with random intitial parameters, neutral evolution with additional protein components and general questions of robustness and evolavability.

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