The effective structure of complex networks drives dynamics, criticality and control

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Abstract

Network Science has provided predictive models of many complex systems from molecular biology to social interactions. Most of this success is achieved by reducing multivariate dynamics to a graph of static interactions. Such network structure approach has provided many insights about the organization of complex systems. However, there is also a need to understand how to control them; for example, to revert a diseased cell to a healthy state or a mature cell to a pluripotent state in systems biology models of biochemical regulation.

Based on recent work [2], using various Boolean models of biochemical regulation dynamics and large ensembles of network motifs, we show that in general the control of complex networks cannot be predicted from structure alone. Structure-only methods such as structural controllability and minimum dominating set theory both undershoot and overshoot the number and which sets of variables actually control these models, highlighting the importance of dynamics in determining control. We show that canalization measured as logical redundancy in automata transition functions models [5] plays a very important role in the extent to which structure predicts dynamics.

To further understand how canalization influences the controllability of multivariate dynamics, we introduce the concept of effective structure, obtained by removing all redundancy from the (discrete) dynamics of models of biochemical regulation using our schemata redescription approach [5]. We show how such effective structure reveals the dynamical modularity [3] and robustness in systems biology models [5]. Furthermore, we demonstrate that the connectivity (i.e. the in-degree) of the effective graph is an order parameter of Boolean Network dynamics, and a major factor in network controllability [4]. Indeed, we propose a new theory for criticality in Boolean networks based on effective connectivity ke (the in-degree of the effective structure), which substantially outperforms the existing theory [1] based on the in-degree of the original connectivity of Boolean networks (see Figure 1 and its caption for details).

References

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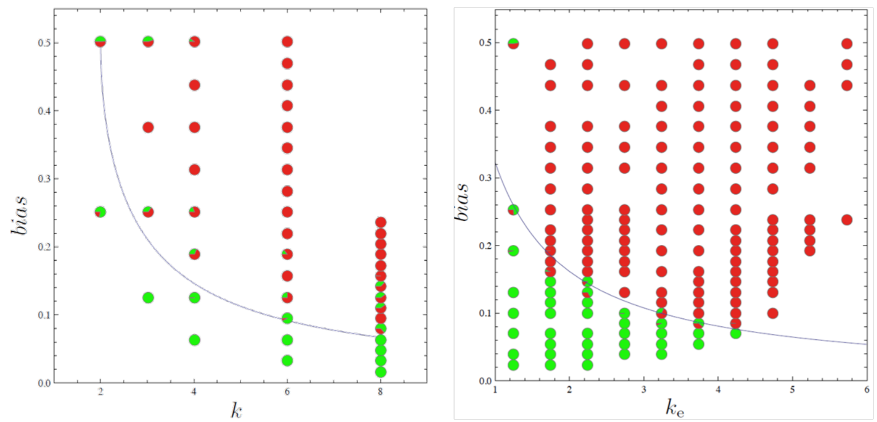

Current Theory (CT): No redundancy is considered, only connectivity and bias of logical functions. Green: stable ensembles of BN. Red chaotic ensembles of BN. Blue line, criticality region for CT.

New Theory (NT): Redundancy is considered as effective connectivity (a form of canalization). Red chaotic ensembles of BN. Blue line, criticality region for NT.

code	equation	acc	f1	mcc	R^2
CT	$crit_{\text{bias}}(k) =, 0.5\left(1-\sqrt{1-\frac{2}{k}}\right)$	0.90	0.75	0.73	0.28
NT	$crit_{\text{bias}}(ke) =, \frac{0.32}{ke}$	0.97	0.97	0.93	0.88

Fig. 1: *Criticality in Boolean Network Ensembles.* Left, current theory [1] for criticality in Boolean networks based on mean in-degree k of network (horizontal) and mean bias of its Boolean functions (vertical). Right, proposed theory [4] based on mean effective connectivity ke (horizontal) and mean bias of Boolean functions (vertical). Data points are denote by pie charts of all Boolean networks in ensemble with respective bias and k or k_e. Red denotes Boolean networks with chaotic dynamics, and green denotes Boolean networks with stable dynamics. In the space of the existing theory, we can observe stable networks well above the predicted criticality line, as well as chaotic networks below this line. Such observations are much rarer in the space of the new theory, which results in substantially higher classification performance after 4-fold cross-validation. For instance, Mathews correlation coefficient (MCC) a performance measure very well suited for unbalanced classification scenarios such as this one is 0.93 for the new theory and 0.73 for the current theory.

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