New Quantification of Local Transition Heterogeneity of Multiscale Complex Networks Constructed from Single-Molecule Time Series

Chun-Biu Li[1], Haw Yang[3,*] & Tamiki Komatsuzaki[1,2]
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([1]Research Institute for Electronic Science, Hokkaido University; [2]JST/CREST; [3]Department of Chemistry, Univer*sity of California at Berkeley)

A new measure, termed "transition complexity", is presented to quantify the local topographical feature, i.e., diversity in transitions from a state to the others, on complex networks. This measure is composed of two contributions: one is related to the number of outgoing links from a state (known as degree) and the other is related to heterogeneity in transition probabilities from a state to the others associated with the links.

To illustrate the potential of the new measure, we apply it to the multiscale state space networks (SSNs) extracted directly from the single molecule time series of protein fluctuation of the NADH:flavin oxidoreductase complex by using a recently developed technique [Li, C. B.; Yang, H.; Komatsuzaki, T. *Proc. Natl. Acad. Sci. U.S.A.* **2008**, *105*, 536]. We find that the multiscale SSN network structures dependent on the time scale of observation are not differentiated significantly in the topological feature of the SSNs where the connectivity pattern among the nodes is solely taken into account, but instead in the weighted properties of the network including the heterogeneous strengths of transitions and the resident probabilities of the nodes (see Fig.1). The relationship of the transition heterogeneity with the anomalous diffusion observed in the single-molecule measurement is also discussed.

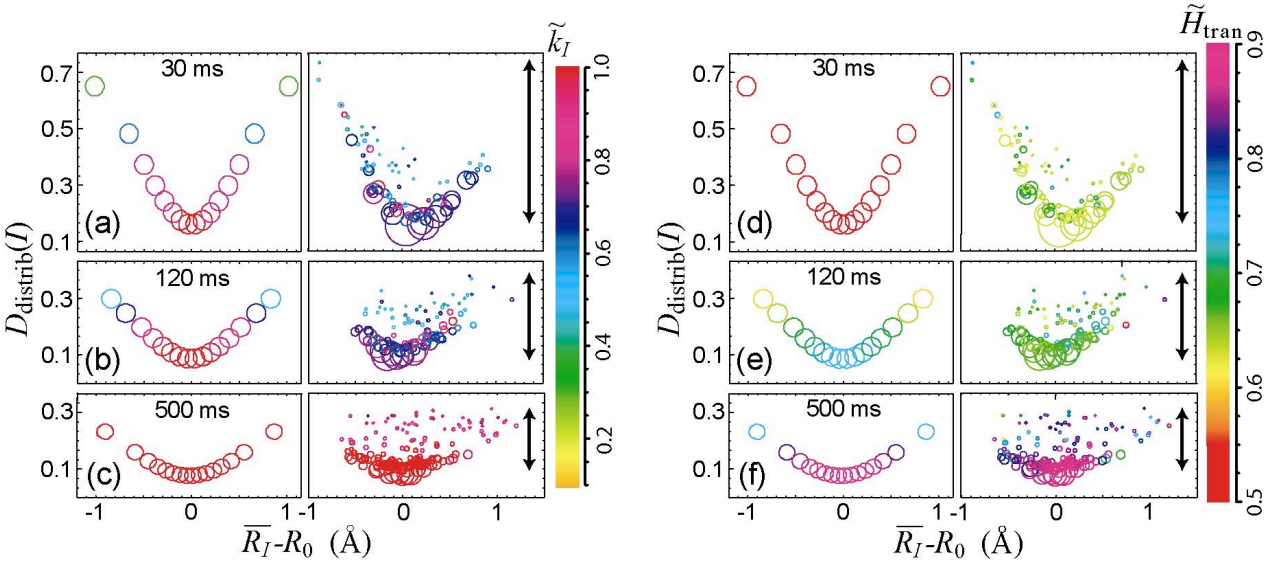

Fig. 1: Dependence of the topographical feature of SSNs for the protein fluctuation timescales of (a, d) 30, (b, e) 120, and (c, f) 500 ms for the NADH:flavin oxidoreductase complex. The abscissa and ordinate denote the average electron donor-acceptor distance and $D_{\mathrm{distrib}}(I)$ (the average distribution distance) associated with the Ith state in each SSN, respectively. In rows (a)-(c), the color coding corresponds to the normalized degree of the SSNs. In rows (d)-(f), the color coding corresponds to the transition entropy. In all panels, the area of the circle is proportional to the resident probability of the state and the arrow indicates the (global) variance of $D_{\mathrm{distrib}}(I)$. For comparison, the corresponding quantities for the overdamped Langevin dynamics (normal diffusion) are shown along the left column.

* Current address: Department of Chemistry, Princeton University