Mapping from Architecture to Dynamics: A Unified View of Dynamical Processes on Networks

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Although it is unambiguously agreed that structure plays a fundamental role in shaping the dynamics of complex systems, this intricate relationship still remains unclear. We investigate a general computational transformation by which we can map the network topology directly to the dynamical patterns emergent on it — independent of the nature of the dynamical process. We find that many seemingly diverse dynamical processes such as coupled oscillators and diffusion phenomena can all be understood and unified through this same procedure. Using the multiscale complexity measure derived from the structure-dynamics transformation, we find that the topological features like hierarchy, heterogeneity and modularity all result in higher complexity. This result suggests a universal principle: it is the desire for functional diversity that drives the evolution of network architecture.

Recent advances in the realm of complex networks have furnished us with a new paradigm to understand and characterize complex systems [1, 2, 3], from the human brain that is composed of billions of interconnected neurons, to our society with six billion cooperating individuals. The discovery of the distinctive scale free [4] and the small world [5] structures has fundamentally altered our view of these networks. A variety of other complex topological features, such as high clustering [6], hierarchical ordering [7], and degree mixing [8], are also emerging as important to the overall behaviour of network systems. However, recent progress has focussed mainly on the underlying topology [9], the effort to unravel the system’s dynamics or function has been less advanced [2, 3, 9]. With the increasing capability to capture simultaneously the time dependent activity of many components in complex systems [10] (such as the multiple electrode recordings and gene expression patterns), unraveling the intricate relationship between the structural and functional characteristics has become a problem of utmost importance, and hints toward generic organizing principles and a deeper understanding of “complexity”. Generally, the topological descriptors fail to explicitly capture the dynamical aspects. In order to characterize the dynamics, one must implement the particular dynamical process on networks via extensive numerical simulations.

In this paper we propose a methodology that allows one to predict the collective dynamics (or functions) of a complex system directly from the underlying topology. Yet, this methodology is independent of the details of dynamical process. This is achieved by constructing node interaction profiles through a kernel function, which quantitatively identify the role of each node in shaping the integrated dynamics and thus captures the way nodes are dynamically interacting with one another. Notably, we find that synchronization of coupled oscillator, ensemble neuron firing, epidemic spreading and diffusion process can all be unified under this theoretical picture, suggesting that some universal mechanisms may govern the overall dynamical behavior of the seemingly diverse complex systems. Based on this transformation we propose a “function-driven” multiscale complexity measure by virtue of the adjustable kernel bandwidth, which unravels the functional organization of a network at different levels. We find that structural complexity measures such as topological heterogeneity [1], modularity [6], hierarchy [7], and nontrivial correlation [8] all translate into higher functional complexity, indicating that the need for multiple function governs the structural evolution of networks.

Consider a complex system of $N$ coupled dynamical units, whose equations are described by [11]:

\[
\dot{x}_i = F(x_i) + \sigma \sum_{j=1}^{N} A_{ij} H(x_j), \quad i = 1, 2, ..., N
\]

where $\dot{x}_i = F(x_i)$ governs the dynamics of each component, $H$ is a fixed output function, $\sigma$ represents the coupling strength, and $A$ is the coupling or adjacency matrix. The problem is now, given the topology $A$ of the network, can we infer qualitatively the dynamics without implementing and computationally simulating it? If so, what does this tell us about the behavior of different dynamical units within the same network structure? By “dynamics” we refer to the pattern of temporal correlations among outputs $x_i(t), i = 1, ..., N$. This has been intensively studied in chaos community and in brain research groups, under either the banner of synchronization [11, 12, 13] or functional connectivity [14].

Obviously, to predict the collective dynamics, we must identify the effective influence of each unit to others, and distinguish their specific, functional roles in shaping the dynamics of each unit. A fundamental feature of com-

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plex interacting systems is the presence of interactions across all scales. To describe the fact that directly coupled components usually exert a stronger influence on each other and the impact attenuation through intermediaries nodes, we adopt a simple, monotonically decreasing function known as a “kernel” $K$. For a pair of nodes $i$ and $j$, we then define their effective interaction $R_{ij}$, in the form of $K(x_{ij}, h)$, where $x_{ij}$ is their shortest distance, $K$ is a non-negative, symmetric kernel function satisfying $\int_R K(x) dx = 1$, $\int_R x K(x) dx = 0$, $\lim_{x \to -\infty} K(x) dx = 0$, and $h$ is the bandwidth that controls the width of the kernel. For Gaussian kernel, the interaction matrix $R$ will read: $R_{ij} = \exp(-x_{ij}^2/2h^2)$.

Note that the $i$-th row of $R$, $R_i$, portrays the effective interaction node $i$ receives from all its neighbors, which we call interaction profile of node $i$. This vectorial profile systematically encodes the identity of all neighbors of node $i$ as distinct driving forces (with different intensities determined by the kernel) to its own dynamics, and does not depend on specific choice of kernels. Therefore $R_i$ defines the unique “status” of node $i$. To further predict the dynamical correlation or functional connectivity $F_{ij}$ between node $i$ and $j$, we can calculate the similarity between their interaction profiles $R_i$ and $R_j$: $F_{ij} = \frac{R_i \cdot R_j}{\|R_i\| \|R_j\|}$.

The similarity $F_{ij}$ provides a unique clue to evaluate the dynamical proximity between the components. Unit $i$ and $j$ subject to a large number of common inputs (up to higher orders) are more likely to behave similarly. In this case, their profiles $R_i$ and $R_j$ will largely coincide by sharing many common entries, leading to a large $F_{ij}$ — approaching 1. Conversely, a pair of units with few common drives tend to be independent and thus have a $F_{ij}$ near 0. A great advantage of this “kernel” formalism lies in the adjustable bandwidth $h$ which can evaluate different levels of function of the network at various topological scales. In the following we will demonstrate how the collective dynamics of various dynamical processes can be predicted using the above mapping from structure $A$ to dynamics (or function) $F$.

We start with synchronization phenomena, which are widely observed in nature and occupy a privileged position in understanding collective behavior in various disciplines. Recently the interplay between a network’s structure and its synchronization dynamics has attracted significant attention. Here we use Kuramoto model defined on various networks as a prototype example. It is governed by $\dot{\theta}_i = \omega_i + \frac{1}{N} \sum_{j=1}^{N} A_{ij} \sin(\theta_j - \theta_i)$, $i = 1, 2, ..., N$, where $\omega_i$ is the frequency of phase oscillators (uniformly distributed in (0,1)), $\sigma$ is the coupling strength, $A$ is the adjacency matrix, and $K$ is the mean degree. Specifically, we will show that $F_{ij}$ obtained at different kernel bandwidth $h$ can provide a good prediction of how the collective dynamics evolves with $\sigma$.

With a small coupling $\sigma$, the oscillators are mostly independent. The dynamical distance between outputs of node $i$ and $j$, defined as $D_{ij} = \langle \theta_i(t) - \theta_j(t) \rangle$ (\theta(t) are wrapped to $[0,2\pi]$ and $\langle \cdot \rangle$ means time average) will be non-zero and constitute a narrow distribution. When $\sigma$ is large, the whole network reaches complete synchronization, and $D_{ij}$ distribution will be a narrow peak again near 0. For intermediate $\sigma$, various functional clusters are formed, with $D_{ij}$ distribution broadening. We find that the $D_{ij}$ distributions at various $\sigma$ are exactly reproduced by $F_{ij}$ using different $h$. At a small $h$, all entries in $R_i$ are almost 0 except the $i$th, meaning each node only has impact on itself. The $R_i$s are mostly orthogonal, thus $F_{ij}$ will centralize at 0. By contrast, the kernel becomes flat at a large $h$, leading every node to exert similar influence on all others. The $F_{ij}$ then concentrates near 1 as all $R_i$s are almost identical. For medium $h$, the distribution of $F_{ij}$ broadens within $[0,1]$ with the peaks corresponding to the formed functional clusters.

These examples show that the kernel bandwidth $h$ is playing a role directly analogous to coupling strength $\sigma$, and $F_{ij}$ offers a good prediction of the collective dynamics $D_{ij}$. To further verify this, we first get $D_{ij}$ by implement phase oscillators on networks (a random network and a modular collaboration network are used here as examples). We then plot the correlation coefficient $\rho$.
between $D_{ij}$ and $1 - F_{ij}$ that is obtained at various $h$, see Fig. 4 (we use $1 - F_{ij}$ because it measures dissimilarity similar to $D_{ij}$, while $F_{ij}$ is a similarity measure). We find that for a given $\sigma$, there is always an optimal kernel bandwidth $h_{\text{max}}$ that attains a maximum similarity between $D_{ij}$ and $1 - F_{ij}$, with $h_{\text{max}}$ being proportional to $\sigma$. The matrices $D_{ij}$ and $1 - F_{ij}$ demonstrate very similar patterns (see Fig. 2), reflected by a large correlation coefficient $\rho$. We find that $\rho$ generally takes a large value for medium and high coupling $\sigma$, where oscillators have self-organized into functional clusters. For weak $\sigma$, the oscillators are largely independent, thus $D_{ij}$ is somewhat random and cannot be accurately fitted by $F_{ij}$.

Now we turn to a concrete example in neuroscience, the coupled neural oscillators in cortex, which communicate by non-smooth, pulse-like firings. The population dynamics of the neurons, like the synchronous firing plays a vital role in cognitive function of the brain. Therefore understanding how connectivity patterns influence the emergent dynamics is of special concern in neuroscience. Here we try to approach the population neuronal dynamics directly from the underlying anatomy. In particular, we couple the FitzHugh-Nagumo neurons through real networks (by excitatory synapse with synaptic conductance $g$) to get $D_{ij}$ and check if it can be predicted by $F_{ij}$. We use two networks possessing key topological properties of the cortex, i.e., small-world, hierarchical and modular structure. One is the neural network of Caenorhabditis elegans whose anatomy has been identified. The other is a hierarchically organized modular network [13] with two hierarchical levels.

![FIG. 3: The correlation coefficient between $D_{ij}$ and $1 - F_{ij}$ for (a) C. elegans network with 297 neurons and each has 14 synaptic couplings on average. (b) Hierarchical network with 480 nodes [13]. Each node has 20 links to the most internal community (formed by 30 nodes), 2 links to the most external community (120 nodes that form four 30-nodes groups), and 1 more link to any other node. See supplement material for the detailed parameters of the FHN neurons.](image)

The synaptic conductance $g$ determines the amplitude of pulse conducted to post-synaptic neurons. It plays the same role as $\sigma$ in coupled phase oscillators. The neurons fire almost randomly with a small $g$, and begin to form synchronous firing as $g$ increases, giving rise to coherent oscillations. We define the collective dynamics of neuron firing as $D_{ij} = \langle |f_i(n) - f_j(n)| \rangle$, where $f_i(n)$ is the number of firings within time window $n$ for neuron $i$. We find that the functional similarity $F_{ij}$ obtained purely from the network structure shows a high correlation with $D_{ij}$ for both the C. elegans and the hierarchical network, see Fig. 3. Therefore we can precisely predict the dynamics of neuronal populations. Moreover, the kernel bandwidth $h$ plays a role similar to synaptic conductance $g$. For a given $g$, there is always an optimal bandwidth $h_{\text{max}}$ under which $F_{ij}$ best fits $D_{ij}$, and this $h_{\text{max}}$ is proportional to $g$.

The above mapping can predict the collective behavior not only for the coupled dynamical systems, but also for the general diffusion process on networks like epidemic spreading [18]. The collective behavior here means the correlation among the epidemic dynamics of the individuals, with the dynamics of node $i$ being a discrete-time stochastic process $S_i(t)$ (1 indicates infected and 0 for healthy). The collective dynamics is then defined as $D_{ij} = \langle |S_i^j(n) - S_j^i(n')| \rangle$, where $S_i^j(n)$ is coarse grained from $S_i(t)$ by counting the number of 1 in time window $n$. We find that $D_{ij}$ is again nicely predicted by $F_{ij}$ under a suitable $h$, see Fig. 4 where we run SIS models on two typical networks. Interestingly, we find $h_{\text{max}}$ relates closely to the effective spreading rate $\lambda = \nu/\delta$, where $\nu$ and $\delta$ are infection and recovery rate of an individual. In Fig. 4 we see that $D_{ij}$ under small and large $\lambda$ is best fitted by a kernel with small and large $h$, respectively. This is because an infected node recovers quickly at a small $\lambda$ and has a small influence range. A large $\lambda$ makes the node persistently infective to even its higher order neighbors, thus is described better by a wider kernel.

![FIG. 4: Correlation coefficient between $D_{ij}$ and $1 - F_{ij}$ for epidemic spreading on (a) scale free BA network (500 nodes with mean degree 5) and (b) email network [10] (1133 nodes).](image)

Having established the mapping from structure to function, we are naturally led to the fundamental problems: why do the various structures such as modularity, hierarchy and degree mixing exist in real networks? What are their roles in shaping the function? Here we
provide an explanation under the framework of complexity by exploiting the above structure-function transformation. Understanding complexity [20][21] has long been a grand challenge that spans a wide variety of fields. Sporns et al. proposed “neural complexity” to measure functional connectivity by implementing Gaussian dynamics [22] on networks. Evolutionarily speaking, the survival of a complex system hinges crucially on the versatility of its function. Inspired by this, we propose to evaluate network complexity by the dynamical patterns it can support. Recall that in coupled oscillators, the evolution of the collective dynamics versus coupling strength are well captured by $H_{ij}$ under various $h$, thus we can approach the function directly through $H_{ij}$. Here we use entropy, defined as $H(F) = \sum p_i \log(p_i)$, to characterize the diversity of $F_{ij}$ obtained at different $h$. We call it multiscale entropy, as it portrays the functional complexity of the network at various topological scales.

In summary we have introduced a novel approach that can map the topological structure of a network directly to its functional organization independent of the details of dynamical processes. Our method not only provides a good prediction of the collective network dynamics, but also allows us to conceptualize the “complexity” of networks through the emergent functions conveniently. This mapping can furthermore be considered as a promising scheme to other problems like inverse engineering and controllability. The explicit relation between structure and function will provide unique clues to infer the structure back from dynamical patterns, possibly with constraints like sparseness of connectivity. The control over the general networked systems can also be expected to enhance conveniently by locating the most sensitive nodes or links, the removal or rewiring of which would result in better network performance.

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FIG. 5: Multiscale entropy for (a) scale free BA, random ER network, assortively and disassortatively mixed BA network. All networks have 1000 nodes and mean degree 20. (b) Hierarchical networks (used in Fig. 3) and (c) Collaboration network [16]. Here we normalize $H$ by a factor $H_m = \log(m)$, which is the entropy for uniform distribution, and $m$ is the bin number.

Now we examine how the intricate topologies can influence the network complexity by computing multiscale entropy. As can be seen in Fig. 5(a), the degree heterogeneity (scale free distribution) and degree mixing [8] (asortive and dissortative) both lead to higher $H$ at various scales, as they promote differentiation or facilitate the formation of modules that can engage into various functions. Remarkably, we find that hierarchical modular networks, which are widely observed in biological and social systems [9], demonstrate notably higher complexity than their random counterparts, see Fig. 5(b) and (c). This is because the multiscale modular structure can provide different levels of function persistently at different scales. The fact that all these distinctive topologies lead to higher functional complexity provides important insights into the evolutionary mechanism of real networks. This suggests a common principle: the demand for functional capability, shapes the network architecture during the development of a physical network.

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