Modular networks emerge from multi-constraint optimization

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Modular structure is ubiquitous among complex networks. To see why such networks evolve towards modular organization we note that they are subject to multiple structural and functional constraints, e.g., minimizing the average path length and the total number of links, while maximizing robustness against perturbations in node activity. We show that the optimal networks satisfying these three constraints are characterized by the existence of multiple sub-networks (modules) sparsely connected to each other. In addition, these modules have distinct hubs resulting in an overall heterogeneous degree distribution, as seen in many real networks.

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Complex networks have recently become a focus of scientific attention, with many natural, social and technological networks seen to share certain universal structural features [1, 2]. These networks often exhibit topological characteristics that are far from random. For instance, they show a significant presence of hubs, i.e., nodes with large degree or number of connections to other nodes. Indeed, hubs are crucial for linking nodes in real networks, which have extremely sparse connectivity, with the probability of connection between any pair of nodes, $C$, varying between $10^{-1} - 10^{-8}$ [1]. A random network with such small $C$ is almost always disconnected. However, a few hubs enable the entire network to be connected, still keeping the total number of links small. These hubs also lead to the “small-world” effect [3] by reducing the average path length of the network. Another property observed in many networks is the existence of a modular structure. We define a network to be modular if it can be decomposed into distinct sub-networks or modules by removing a few links. Such networks exhibit significantly more intra-modular connections compared to inter-modular connections. Modular networks observed in empirical studies span a wide range from cellular networks involved in metabolism and signalling [4, 5, 6, 7], to cortical networks [8], social networks [9], food webs [10] and the internet [11]. Many of these networks also exhibit large number of hubs, which often have the role of interconnecting different modules [12].

The majority of previous studies on modular networks have been concerned with methods to identify community structure of a network [13]. There have been relatively few attempts to explain the potentially more interesting question of how and why modularity emerges in complex networks. Most such attempts are based on the notion of evolutionary pressure, where a system is driven towards a modular architecture by the need for adapting to changing environment [14, 15]. However, such explanations involve complicated adaptive mechanisms, in which the environment itself is assumed to change in a modular fashion. Further, adaptation might lead to decrease in connectivity through biased selection of sparse networks, which eventually results in disruption of the network with the modules being isolated nodes [14] or disconnected parts [10].

A crucial limitation of these above studies is that they almost always focus on a single performance parameter. However, in reality, most networks have to optimize between several, often conflicting, constraints. While structural constraints, such as path length, had been the focus of initial work by network researchers, there has been a growing realization that most networks have dynamics associated with their nodes [17]. The robustness of network behavior such as synchronized dynamical states, is often vital to the efficient functioning of many systems, and also imposes an important constraint on networks. Therefore, the role played by dynamical considerations in determining the topological properties of a network is a challenging and important question that opens up new possibilities for explaining observed features of complex networks. In this letter, we propose a simple mechanism for the emergence of modularity in networks as an optimal solution for satisfying a minimal set of structural and functional constraints. These essentially involve (i) reducing the average path length, $\ell$, of a network by (ii) using a minimum number of total links, $L_{total}$, while (iii) ensuring the stability of dynamical states associated with the network.

We investigate the dynamical stability of a network by measuring the rate at which a small perturbation about an equilibrium state of the network dynamics grows with time. This is determined by the largest real part $\lambda_{max}$ of the eigenvalues for the Jacobian matrix $J$ representing the interactions among the nodes [18]. The system is stable if $\lambda_{max} < 0$, and unstable otherwise. The matrix elements $J_{ij}(\sim A_{ij} W_{ij})$ include information about both the topological structure of the network, given by the adjacency matrix $A$ ($A_{ij}$ is 1, if nodes $i, j$ are connected, and 0, otherwise), as well as, the distribution of interaction strengths $W_{ij}$ between nodes. In our simulations, $W_{ij}$ has a Gaussian distribution with zero mean and variance $\sigma^2$; however, a non-zero mean does not qualitatively change our results. For an Erdős-Rényi (ER) random network, $J$
is a sparse random matrix, with \( \lambda_{\text{max}} \sim \sqrt{NC\sigma^2} - 1 \), according to the May-Wigner theorem \[\text{(19)}\]. Increasing the system size \( N \), connectivity \( C \) or interaction strength \( \sigma \), results in a transition from stability to instability for the dynamical state of the network. This result has been shown to be remarkably robust with respect to various generalizations \[\text{(20)}\].

Networks are also subject to certain structural constraints. One of them is the need to save resources, manifested in minimizing link cost, i.e., the cost involved in building and maintaining each link in a network \[\text{(21)}\]. This results in the network having a small total number of links, \( L_{\text{total}} \). However, such a procedure runs counter to another important consideration for networks, namely, reducing the average path length \( \ell \), which improves its efficiency by increasing the communication speed among the nodes \[\text{(22)}\]. The conflict between these two criteria can be illustrated through the example of airline transportation networks. Although, fastest communication (i.e., small \( \ell \)) will be achieved if every airport is connected to every other through direct flights, such a system is prohibitively expensive as every route involves some cost in maintaining it. In reality, therefore, one observes the existence of airline hubs, which act as transit points for passengers arriving from and going to other airports.

For ER random networks, although \( \ell \) is low, \( L_{\text{total}} \) is high because of the requirement to ensure that the network is connected: \( L_{\text{total}} > N \ln N \) \[\text{(24)}\]. Introducing the constraint of link cost (i.e., minimizing \( L_{\text{total}} \)) while requiring low average path length \( \ell \), leads to a star-like connection topology (Fig. \( \text{1C} \)). We define a star network as one with a single hub to which all other nodes are connected, there being no other links. Its average degree \( \langle k \rangle \approx 2 \) is non-extensive with system size, and is much smaller than a connected random network, where \( \langle k \rangle \sim \ln N \).

However, such star-like networks are extremely unstable with respect to dynamical perturbations in the activity of their nodes. The probability of dynamical instability in random networks increases only with average degree \( \lambda_{\text{max}} \sim \sqrt{\langle k \rangle} \), since \( \langle k \rangle = NC \), while for star networks it increases with the largest degree, and hence the size of the network itself \( \lambda_{\text{max}} \sim \sqrt{N} \). To extend this for the case of weighted networks we look at the largest eigenvalue of \( J \), \( \lambda_{\text{max}} = -1 + \sqrt{\sum_{i=2}^{N} J_{ii}J_{1i}} \), the hub being labeled as node 1. The stability of the weighted star network is governed by \( \sum_{i=2}^{N} J_{ii}J_{1i} \), which is the displacement due to a 1-dimensional random walk of \( N - 1 \) steps whose lengths are products of pairs of random numbers chosen from a Normal \((0, \sigma^2)\) distribution.

To obtain networks which satisfy the dynamical as well as the structural constraints we perform optimization using simulated annealing, with a network having \( N \) nodes and \( N - 1 \) links (the smallest number that would allow the network to be connected). Having fixed \( L_{\text{total}} \), the energy function to be minimized is defined as

\[
E(\alpha) = a\ell + (1 - \alpha)\lambda_{\text{max}},
\]

where \( 0 \leq \alpha \leq 1 \) is the parameter that denotes the relative importance of the path length constraint with respect to the condition for dynamical stability. At each step a rewiring is done and the update is (i) rejected if the updated network is disconnected, (ii) accepted if \( \delta E = E_{\text{final}} - E_{\text{initial}} < 0 \), and (iii) if \( \delta E > 0 \), then accepted with probability \( p = \exp(-\delta E/T) \), where \( T \) is the “temperature”. The initial temperature was chosen in such a way that energetically unfavorable moves had 80% chance of being accepted. After each monte carlo step \( (N \) updates) the temperature was reduced by 1% and iterated till there was no change in the energy for 20 successive monte carlo steps. For each value of \( \alpha \), the optimized network with lowest \( E \) was obtained from 100 realizations. The results for \( N = 64 \) are shown in Fig. \( \text{1} \).

As can be seen from Fig. \( \text{1} \) modularity emerges when the system tries to satisfy the twin constraints of minimizing \( \ell \) as well as \( \lambda_{\text{max}} \). When \( \alpha \) is very high \( (\sim 0.8) \) such that the dynamical stability criterion becomes less important, the system shows a transition to a star-like configuration with a single hub. However, as \( \alpha \) is decreased, the instability of the hub makes the network less preferable and for intermediate values of \( \alpha \), the optimal network gets divided into modules, as seen from the mea-
marked by functional constraints we look at the change in stability behavior of the degree entropy, modular and star structures is further emphasised in the isolated module, the entire system of between the corresponding hubs. The largest eigenvalue for between non-hub nodes, resulting in higher clustering. The larger value of $\lambda$ increases significantly while still satisfying the structural constraints. We now relax the constraint on three constraints are necessary for modularity to emerge runs counter to the general belief that modularity necessarily follows from the requirement of robustness alone, as modules are thought to limit the effects of local perturbations in a network. To further demonstrate that the three constraints are the minimal required for a network to adopt a modular configuration, we remove the hub from a clustered star while ensuring that the network is still connected. This corresponds to the absence of the

FIG. 2: Probability distribution of $\lambda_{\text{max}}$ for a clustered star network ($N = 256, L_{\text{total}} = 15N$) with different numbers of modules ($m$) of equal size and modules connected by single link between the respective hubs. Link weights $J_{ij}$ follow a Normal $(0, \sigma^2)$ distribution with $\sigma^2 = 0.018$. (Inset) Probability of stability $[P(\lambda_{\text{max}}) > 0]$ varying with $\sigma^2$. Increasing $m$ results in the transition to instability occurring at higher values of $\sigma^2$, implying that network stability increases with modularity.

FIG. 3: Probability distribution of $\lambda_{\text{max}}$ for clustered star networks ($N = 256, L_{\text{total}} = 15N$) having four modules with different types of inter-modular connectivities (A), (B) and (C) described in the text. Link weights $J_{ij}$ have a Normal $(0, \sigma^2)$ distribution with $\sigma^2 = 0.018$. The effect of increasing the number of modules, $m$, on the dynamical stability of a network can be observed from the stability-instability transition that occurs on increasing the network parameter $\sigma$ keeping $N, C$ fixed. We find that the critical value at which the transition to instability occurs, $\sigma_c$, increases with $m$ (Fig. 2 inset) while $\ell$ does not change significantly. This signifies that even for higher values of $L_{\text{total}}$, networks satisfy the structural and functional constraints by adopting a modular configuration.

As $L_{\text{total}}$ is increased, we observe that the additional links in the optimized network occur between modules, in preference to, between nodes in the same module. To see why the network prefers the former configuration, we consider three different types of inter-modular connections: (A) only the hub nodes of different modules are connected, (B) non-hub nodes of one module can connect to the hub of another module, and (C) non-hub nodes of different modules are connected. Arrangement (B) where inter-modular connections that link to hubs of other modules actually increase the maximum degree of the modules, making this arrangement less stable than (A). On the other hand, (C) connections between non-hub nodes of different modules not only increase the stability (Fig. 3), but also reduce $\ell$. As a result, the optimal network will always prefer this arrangement (C) of large number of random inter-modular connections over other topologies for large $L_{\text{total}}$.

Our observation that both structural and dynamical constraints are necessary for modularity to emerge runs counter to the general belief that modularity necessarily follows from the requirement of robustness alone, as modules are thought to limit the effects of local perturbations in a network. To further demonstrate that the three constraints are the minimal required for a network to adopt a modular configuration, we remove the hub from a clustered star while ensuring that the network is still connected. This corresponds to the absence of the

\[ H = -\sum_k p_k \ln p_k, \]  

where $p_k$ is the probability of a node having degree $k$. The emergence of a dominant hub at a critical value of $\alpha$ is marked by $H$ reducing to a low value.

To understand why modular networks emerge as the solution for simultaneous optimization of structural and functional constraints we look at the change in stability that occurs when a star network is split into $m$ modules, with each module connected to others through links between the corresponding hubs. The largest eigenvalue for the entire system of $N$ nodes is the same as that for each isolated module, $\lambda_{\text{max}} \sim \sqrt{N/m}$, as the additional effect of the few inter-modular links is negligible. At the same time, the increase in the average path length $\ell$ with $m$ is almost insignificant. Therefore, by dividing the network into a connected set of small modules, each of which is a star sub-network, the stability of the entire network increases significantly while still satisfying the structural constraints.

The above results were obtained for a specific value of $L_{\text{total}}$ ($= N - 1$). We now relax the constraint on link cost by allowing a much larger number of links than that strictly necessary to keep the network connected. The larger value of $L_{\text{total}}$ is manifested as random links between non-hub nodes, resulting in higher clustering within the network. For such clustered star networks also, $\lambda_{\text{max}}$ increases with size as $\sqrt{N}$, and therefore, their stability is enhanced by imposing a modular structure.
In this paper we have shown that modules of interconected nodes can arise as a result of optimizing between multiple structural and functional constraints. In particular, we show that by minimizing link cost as well as path length, while at the same time increasing robustness to dynamical perturbations, a system of nodes will evolve to a configuration having multiple modules characterized by hubs, that are connected to each other. At the limit of extremely small $L_{\text{total}}$ this results in networks with bimodal degree distribution, that has been previously shown to be robust with respect to both targeted and random removal of nodes [26]. Therefore, not only are such modular network dynamically stable, but they are also robust with respect to structural perturbations.

In general, when allowing larger $L_{\text{total}}$, the optimized networks show heterogeneous degree distribution that has been observed in a large class of networks occurring in the natural and social world, including those termed as scale-free networks [2]. Our results provide a glimpse into how the topological structure of complex networks can be related to functional and evolutionary considerations.

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[18] The diagonal elements $J_{ii} = -1$, so we only consider instability induced through the network couplings.