Sampling motif-constrained ensembles of networks

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The statistical significance of network properties is conditioned on null models which satisfy specified properties but that are otherwise random. Exponential random graph models are a principled theoretical framework to generate such constrained ensembles, but which often fail in practice, either due to model inconsistency, or due to the impossibility to sample networks from them. These problems affect the important case of networks with prescribed clustering coefficient or number of small connected subgraphs (motifs). In this paper we use the Wang-Landau method to obtain a multicanonical sampling that overcomes both these problems. We sample, in polynomial time, networks with arbitrary degree sequences from ensembles with imposed motifs counts. Applying this method to social networks, we investigate the relation between transitivity and homophily, and we quantify the correlation between different types of motifs, finding that single motifs can explain up to 60% of the variation of motif profiles.

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I. INTRODUCTION

Networks form the basis of an ample class of complex systems. The observed topological patterns of such systems often yield the only available evidence for the underlying principles behind their formation. However, the significance of any observed property can only be assessed in comparison to a properly defined network ensemble that acts as a “null” model [1–3]. For instance, clustering (i.e. high density of triangles), skewed degree distributions, and community structure are considered significant in real networks because they are absent in Erdős-Rényi networks. To perform such comparisons, it is essential not only to properly define such null models, but also to correctly sample network realizations from them. This is relatively straightforward when the ensemble generates networks where the edges are sampled independently (e.g. Erdős-Rényi and configuration models [4, 5], the stochastic block model [6, 7]) and it remains feasible when strict edge independence is violated due to hard constraints [8, 10]. However, for ensembles with more generic constraints the sampling is significantly more challenging. A particularly important example are ensembles with a prescribed density of connected subgraphs (“motifs”) [11–13]. For this class of models, one often finds abrupt phase transitions, where sampled networks possess either very high or very low motif density [12, 13], excluding intermediary values often encountered in real systems. Furthermore, they often show strong non-ergodic behavior, with very slow relaxation that forbids unbiased sampling in practical computational time [13]. Since the edge placement is not independent, the densities of different motifs are correlated with each other and also with large-scale network structures [14, 15]. Without addressing the issue of correct sampling, these correlations cannot be properly identified, which makes the occurrence of these patterns in real systems difficult to interpret. In particular, it is not possible to conclude whether a particular motif density profile indicates a topology optimized towards robustness [16, 17] or whether it is merely a byproduct of a specific large-scale structure [14, 18] or of correlations between motifs.

In this paper we show how to sample from ensembles with prescribed motif densities in polynomial time. We employ a multicanonical Monte Carlo method [19] that allows the entire range of the order parameter to be explored. In this manner, not only the non-ergodicity problem is explicitly avoided, but it also becomes possible to sample networks with arbitrary motif densities, even those at intermediate values that are unattainable via traditional importance sampling. This allow us to quantitatively investigate two fundamental problems in social networks: the homophily-transitivity relationship and the interdependence of different motif types.

II. SAMPLING METHODS

We are interested in network ensembles that possess one particular observable s of interest, but that are otherwise maximally random. Both these features are achieved by sampling the network from an exponential random graph model (ERGM) [3, 10, 21–24] G, where each graph g ∈ G occurs with probability

\[ \Pi_\beta(g) = \frac{e^{\beta s(g)}}{Z_\beta}, \]

where \( Z_\beta = \sum_{g \in G} e^{\beta s(g)} \),

where \( s(g) \) is the observable associated with network \( g \), and \( \beta \) is an inverse-temperature parameter, in analogy to the canonical ensemble in statistical physics. The distribution of \( s \) is \( \rho_\beta(s) = \sum_{g \in G} \delta(s(g) - s)\Pi(g) = \rho_0(s)e^{\beta s} \), where \( \rho_0(s) \equiv \rho_{\beta=0}(s) \) is called the state density. For a given value of \( \beta \), the ensemble average \( \langle s \rangle_\beta \equiv \sum_s s \rho_\beta(s) \) attains a specific value, and hence the ensemble serves as a null model for networks with \( s(g) = \langle s \rangle_\beta \). The number
As an alternative to the canonical sampling described above, we propose a multicanonical sampling to overcome the aforementioned problem. This method aims to sample networks uniformly on a pre-defined observable range \([s_{\text{min}}, s_{\text{max}}]\), thus overcoming minima of \(\rho_0(s)\). This is done by sampling the states according to auxiliary ensemble with probabilities \(\Pi'(g) \propto 1/\rho_0(s(g))\), achieved by simply changing the acceptance to \(A(g \rightarrow g') = \min\{1, \rho_0(s(g'))/\rho_0(s(g))\}\) \([19]\). However, in order to perform this sampling we need to know the state density \(\rho_0(s)\). After convergence, the estimate of \(\rho_0(s)\) allows for the computation of \(\rho_3(s)\) for all \(\beta\) using \(\rho_3(s) = \rho_0(s) \exp(\beta s)\). Hence, the auxiliary ensemble allows to explore the original canonical ensembles without being restricted to the most probable regions. More importantly, we can impose the desired value of the observable as a hard constraint a posteriori, i.e., only sample networks with \(s(g) = s^*\). The multicanonical approach has recently been applied to investigate the spectral gap of networks \([28]\) and related approaches have been used to investigate percolation \([29]\) and resilience properties of networks \([30]\).

III. APPLICATION TO K-REGULAR NETWORKS

In Fig. 1 we show how the application of multicanonical sampling solves the limitations of canonical sampling in the classical problem of introducing clustering in a k-regular network \([11, 13]\). Here, nodes are forced to have the same degree \(k\) and the observable of interest is the number of triangles, \(s(g) = n_\Delta\). Fixing \(n_\Delta\) is the same as fixing the clustering coefficient \(c = 3n_\Delta/n_c\), where \(n_\Delta\) is the number of connected triples (a constant for all networks with the same degree sequence) \([3]\). This model exhibits a transition at a specific value of \(\beta = \beta_{PT} \approx 3.54\) for \(k = 4\), separating low and high-clustering phases \([13]\). The canonical sampling is unable to compute \(\langle c \rangle\) close to the phase-transition it yields different estimations of \(\langle c \rangle\), depending whether \(\beta\) is slowly increased (\(\beta \uparrow\), lower branch) or decreased (\(\beta \downarrow\), upper branch). This hysteresis is typical around first-order phase transitions (coexisting phases) and indicates that the canonical sampling is in a metastable state. Indeed, \(\rho_3\) has two local maxima in which the canonical sampling becomes trapped (inset in Fig. 1). On the other hand, the multicanonical sampling is immune to these problems: it correctly characterizes \(\langle c \rangle\) at \(\beta = \beta_{PT}\) and reveals the full distribution \(\rho_3(\beta_{PT})\).

Hence, the method is not only capable of computing the correct ensemble average for any \(\beta\), it yields typical networks with any value of \(c\), including the significant gap \(c\in[2,1]\) which is unattainable with the canonical sampling. In Fig. 2 we confirm that the computational cost of the multicanonical method scales polynomially with system size, a dramatic improvement.
IV. APPLICATION TO REAL NETWORKS

Next we use the multicanonical method to investigate two important problems of social networks. The first problem we consider is to distinguish between homophily (the tendency of “similar” nodes to connect to each other) and transitivity (the tendency of nodes that already share a common neighbor to connect to each other) in social networks [2, 14, 33, 39]. We use the (undirected) network of email exchange within a university [32]. It consists of $N=1,133$ users, and $M=5,451$ email exchanges, and a roughly exponential degree distribution. As observables we consider the clustering coefficient $c$ and the degree assortativity $r$ [27], for which we obtain $c^*=0.166(12)$ and $r^*=0.08(3)$ (uncertainties in the last digit estimated using the order-10 Jackknife method). We assess the significance of these values by comparing them to those obtained in the following three network ensembles with the same degree sequence as in the original network:

(i) Same weight to all networks $g$ (i.e. the configuration model). Canonical sampling with $\beta=0$ yields $\langle c \rangle_{\beta=0}=0.028(1)$ and $\langle r_{\beta=0} \rangle=0.017(13)$, much smaller than $c^*$ and $r^*$ as typically found in social networks.

(ii) ERGMs with $\langle c \rangle = c^*$. These ensembles clarify the interdependence of $r$ and $c$. In particular, in order to determine whether the assortativity is a consequence of high clustering [14] we would like to measure $\langle r \rangle$ from the null model with $\langle c \rangle = c^*$. This canonical sampling fails because $\langle c \rangle_{\beta} vs. \beta$ shows an hysteresis around $s=c^*$ (inset of Fig. 2 in agreement with our previous discussion).

(iii) Hard constraints with $c(g) = c^*$, obtained using multicanonical sampling. As mentioned before, this type of hard constraint is unfeasible with canonical sampling, even if the desired observable value is realizable. With the multicanonical method we sample points after a number of Monte Carlo steps proportional to the tunneling time, which guarantees that the sampled points are independent and unbiased [20]. We performed multicanonical sampling for a desired $c$ and measured the assortativity $r$. The results are shown in Fig. 3 and reveal that random networks with the same clustering of the email network $c = c^*$ typically show a much larger assortativity $\langle r \rangle > r^*$. Therefore, although both $c^*$ and $r^*$ are larger than one would expect for a fully random network, the actual value of $r^*$ is significantly less than one would expect by knowing only $c^*$. From this we conclude that transitivity cannot be the only mechanism responsible for the observed degree homophily.

The second problem we address is the extent to which the occurrence of different motifs (connected subgraphs) are related to each other and the impact of such correlations on the so-called motif profiles [17]. Here we focus on directed networks, and the observable of interest is the number $n_i$ of occurrences of a specific motif $i$. Again, traditional sampling methods are not suited to address this problem because of the existence of (potentially multiple [13]) discontinuous phase transitions. Instead, using...
FIG. 4. (Color online) Motifs are correlated to each other in blocks. (a) The Pearson correlation coefficient \( R_{ij} = \langle (n_i - \langle n_i \rangle)(n_j - \langle n_j \rangle) \rangle / \sigma_i \sigma_j \), between motifs \( i \) and \( j \), computed by varying the constrained motif (in a range which includes the values of the real and random networks, Fig. 3). (b) Upper panel: Motif profile [17] built from the z-score \( z \) vs. \( j \) \((z_j = (n_j - \langle n_j \rangle) / \sigma_j)\), where \( n_j \) is the number of motifs \( j \) and \( \langle \ldots \rangle \) and \( \sigma_j \) are the average and standard deviation in the \( \beta = 0 \) ensemble. Different lines correspond to the \( z_j \) of the real network (\( z_j^* \), blue line) and the expected \( z_j \)'s in the constrained ensemble in which \( n_i \) is equal to the \( n_i^* \) of the real network, where \( i \) is the constrained motif shown in the legend \((z_j = z_j^* \text{ for } j = i)\). Middle panel: the correlation between the profiles shown in the upper panel, i.e., between the profile \( z \) of the real network and the profile \( z' \) of the motif-i constrained network (as a function of \( i \)), computed as \( R_{z,z'} = \langle (z z') \rangle - \langle z \rangle \langle z' \rangle / \sigma_z \), where \( \langle \ldots \rangle \) and \( \sigma_z \) were computed over \( j \neq i \). Lower panel: comparison of the z-score shown in the upper panel (blue line) and the alternative z-score obtained computing \( \langle \ldots \rangle \) and \( \sigma_j \) in the ensemble constrained by \( n_i = n_i^* \), where \( i \) is indicated in the legend \((z_j \equiv 0 \text{ for } j = i)\).

In summary, we have shown that multicanonical sampling allows for an improved network generation and for the investigation of problems which were otherwise intractable. In particular, we characterize ERGMs in cases where the usual canonical sampling fails and we sample networks imposing hard constraints, an alternative to a direct sampling of ERGMs even when the usual algorithms are feasible. Our analysis of empirical networks demonstrates that using the multicanonical sampling allows the investigation of the interdependence between network properties. In particular, we quantified the correlation between clustering and assortativity, and between different motifs, as well as the extent to which their significance profiles can be explained by single motifs. This opens the possibility of investigating the correlation between motifs as well as other local-scale properties and the large-scale structure of networks [14], such as communities, core-peripheries and many others. The systematic disentangling of these diverse features is a crucial and open problem in the identification of fundamental models of network formation.

V. CONCLUSIONS

In summary, we have shown that multicanonical sampling allows for an improved network generation and for the investigation of problems which were otherwise intractable. In particular, we characterize ERGMs in cases where the usual canonical sampling fails and we sample networks imposing hard constraints, an alternative to a direct sampling of ERGMs even when the usual algorithms are feasible. Our analysis of empirical networks demonstrates that using the multicanonical sampling allows the investigation of the interdependence between network properties. In particular, we quantified the correlation between clustering and assortativity, and between different motifs, as well as the extent to which their significance profiles can be explained by single motifs. This opens the possibility of investigating the correlation between motifs as well as other local-scale properties and the large-scale structure of networks [14], such as communities, core-peripheries and many others. The systematic disentangling of these diverse features is a crucial and open problem in the identification of fundamental models of network formation.

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FIG. 5. (Color online) Co-dependence between motifs in a directed social network (Physicians). The diagonal plots \((i = j)\) show the probability of observing the motif \(i\) in the ensemble of random networks with the same degree distribution (state density). Vertical lines indicate the expected number of motifs (close to the maximum) and the number observed in the real network. The non-diagonal plots show the number of motifs \(n_i\) and \(n_j\) in random networks with fixed number of \(n_i\) (constrained motif). For each constrained motif \(i\), a multicanonical sampling was performed in the range shown in the plot. For each value of the motif \(i\) (vertical axis) in this range, independent samples of networks were recorded and the number of the unconstrained motifs \(j\) (horizontal axis) was measured. The (Pearson) correlation between these values is shown in Fig. 4(a). The motif-profile in Fig. 4(b) was obtained over the values of motifs \(j\) obtained fixing motif \(i\) to the value of the real network.