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Flow graphs: Interweaving dynamics and structure

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The behavior of complex systems is determined not only by the topological organization of their interconnections but also by the dynamical processes taking place among their constituents. A faithful modeling of the dynamics is essential because different dynamical processes may be affected very differently by network topology. A full characterization of such systems thus requires a formalization that encompasses both aspects simultaneously, rather than relying only on the topological adjacency matrix. To achieve this, we introduce the concept of flow graphs, namely weighted networks where dynamical flows are embedded into the link weights. Flow graphs provide an integrated representation of the structure and dynamics of the system, which can then be analyzed with standard tools from network theory. Conversely, a structural network feature of our choice can also be used as the basis for the construction of a flow graph that will then encompass a dynamics biased by such a feature. We illustrate the ideas by focusing on the mathematical properties of generic linear processes on complex networks that can be represented as biased random walks and their dual consensus dynamics, and show how our framework improves our understanding of these processes.

I. INTRODUCTION

The last decade has witnessed an explosion in the number of metrics for the characterization of complex networks [1,2]. Most of these quantities rely on the analysis of topological properties and are, in a sense, combinatorial as they count certain motifs, e.g., edges, triangles, shortest paths, etc. Since these kinds of measures do not account for patterns of flow on the network, flow-based metrics have also been proposed [3–8] and shown to provide new insights, especially in directed networks. However, these metrics usually have the limitation of being defined for discrete-time, unbiased random walks, which might not represent a good description for the process taking place on the graph under scrutiny. Among the systems where unbiased random walks are not realistic, let us mention the Internet and traffic networks, where a bias is necessary to account for local search strategies and navigation rules [9–13]. Whenever complex interdependences between network subunits are generated by patterns of flow [8], e.g. information in social networks or passengers in airline networks, neglecting or misinterpreting the dynamics taking place on the graph leads to an incomplete and sometimes misleading characterization of the system.

The main purpose of this work is to develop a mathematical framework that allows us to analyze the structure of complex networks also from a dynamical point of view. To do so, we focus on a broad range of linear processes, namely biased random walks and consensus dynamics. We show how to define an alternative representation of the graph, called *flow graph*, which naturally embeds flows in the weight of the links and on which dynamical processes become unbiased. In this way, to the same topological graph, one can associate many different flow graphs, each specific of the different dynamics under consideration. This emphasizes the idea that the same

original graph may exhibit different patterns of flow depending on the underlying dynamics, and that the choice of a metric as well as the extraction of pertinent information from a network should be made according to the nature of the dynamical process actually taking place on it.

In the following, we focus on undirected networks $\mathcal{G}$, which are described by their $N \times N$ symmetric adjacency matrix A, where N is the number of nodes. By definition, A_{ij} is the topological weight of the edge going from j to i. The strength $s_i = \sum_j A_{ij}$ of node i is the total weight of the links connected to it. If the network is unweighted, s_i is simply the degree of node i. $W = \sum_{ij} A_{ij}/2$ is the total weight in the network. Whereas the adjacency matrix reflects the underlying topology, nothing so far determines the dynamical processes operating on the system [3]. Here, we consider a broad class of linear processes defined by the equation

$$x_{i;t+1} = \sum_j B_{ij} x_{j;t}, \tag{1}$$

where the evolution of a quantity x_i, associated with node i, is driven by B_{ij}, a matrix related to the adjacency matrix A_{ij}. In particular, in the following we will focus on two subclasses of Eq. (1), namely *random walks* and *consensus problems*.

II. FLOW GRAPHS FOR GENERAL RANDOM WALKS

We start our discussion with dynamical processes aimed at modeling the diffusion of some quantity or information on $\mathcal{G}$. The simplest process we can consider is a discrete-time, unbiased random walk (URW) where, at each step, a walker located at a node j follows one of the links of j with a probability proportional to its weight. In this case, the expected

density of walkers at node i, denoted by p_i, evolves according to the rate equation

$$p_{i;t+1} = \sum_j T_{ij} p_{j;t}, \qquad (2)$$

where T is the transition matrix whose entry T_{ij} represents the probability of jumping from j to i:

$$T_{ij} = A_{ij}/s_j. \qquad (3)$$

In order to preserve the total number of walkers, T_{ij} satisfies the condition of being column normalized, i.e., $\sum_i T_{ij} = 1$. Consequently, $\sum_i p_{i;t} = 1$ is verified for every t. The dynamical process [Eq. (2)] with the transition matrix [Eq. (3)] is known to converge to the equilibrium solution $p_i^* = s_i/2W$ if the graph is connected and nonbipartite, i.e., if the dynamics is ergodic [14].

A. Biased random walks

There exist infinitely many other ways to define a random walk and thus to model diffusion on the same graph $\mathcal{G}$. An interesting class of processes is biased random walks (BRWs), defined as follows [15]. Let each node i be given a definite positive attribute α_i. Then a walker located at node j decides to jump onto one of its neighbors, say i, with a probability proportional to $\alpha_i A_{ij}$. Hence, the probability of jumping from j to i is given by

$$T_{ij}^{(\alpha)} = \frac{\alpha_i A_{ij}}{\sum_k \alpha_k A_{kj}}. \qquad (4)$$

This is equivalent to saying that the motion of a walker is biased according to the values of α associated with the nodes. The attribute α_i can be either a topological property of node i, such as its strength s_i or its betweenness centrality, or, more in general, can represent an arbitrary function of an intrinsic node property, as for instance, the reputation of a person in a social network. For different α, BRWs correspond to distinct diffusive processes characterized by different spectral properties for Eq. (4).

Let us show that it is always possible to interpret the BRW defined by Eq. (4) as an URW on an opportunely defined flow graph $\mathcal{G}'$.[1] This observation has important implications, as it makes possible to use theoretical results known for URWs for the analysis of BRWs. In addition to this, as we will develop below, this representation supplies an alternative, advantageous way to highlight dynamical characteristics of the system. Let us define the nonnegative and symmetric matrix

$$A_{ij}' = \alpha_i A_{ij} \alpha_j. \qquad (5)$$

This is the adjacency matrix of the *flow graph* $\mathcal{G}'$, whose edges are the same as in $\mathcal{G}$ but with different weights (see Fig. 1). It is straightforward to show that an URW on $\mathcal{G}'$, described by the equation $p_{i;t+1}' = \sum_j T_{ij}' p_{j;t}'$ with $T_{ij}' = A_{ij}'/s_j'$, coincides with a BRW on $\mathcal{G}$ driven by the transition matrix [Eq. (4)], since $T_{ij}^{(\alpha)} \equiv T_{ij}'$. This observation implies that the equilibrium
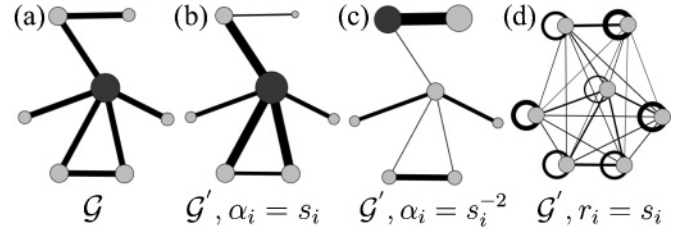
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[1]This result also holds for BRWs where a symmetric attribute $\alpha_{ij} = \alpha_{ji}$ is assigned to edges instead of to nodes.

FIG. 1. Visual representation of (a) an unweighted graph $\mathcal{G}$ and of its flow graphs $\mathcal{G}'$ defined for BRWs with attributes (b) $\alpha_i = s_i$ and (c) $\alpha_i = s_i^{-2}$, and (d) a continuous-time random walk with $t = 2, r_i = s_i$. The width of the links is proportional to their weight, and the surface of the nodes to their strength. The strength leader, i.e., the node with the highest strength, is darkened if it exists. In order to make the graphs comparable, we renormalized the weights in order to ensure that $W = W'$. These examples clearly show that different dynamics lead to different patterns and that important nodes for one dynamics might be less important for other dynamics.

solution $p_j^{*'}$ of the BRW on the original graph, i.e., the dominant eigenvector of Eq. (4), is simply given by the strength of node j in $\mathcal{G}'$:

$$p_j^{*'} = \frac{s_j'}{2W'} = \frac{\sum_i \alpha_i A_{ij} \alpha_j}{\sum_{i,j} \alpha_i A_{ij} \alpha_j}, \qquad (6)$$

in agreement with [15], and can thus be calculated by using only local information of j in $\mathcal{G}'$. This result also shows that A_{ij}' is proportional to the flow of probability from j to i at equilibrium.

In order to illustrate these concepts, let us focus on a class of BRWs where α_i has a power-law dependence on the strength, $\alpha_i = s_i^\gamma$. This functional dependence has been proposed by several authors in order to model local routing strategies [9,10,15]. By changing the exponent γ, one tunes the dependence of the bias on the strength. When $\gamma = 0$, the standard URW is recovered, while biases toward high (low) strengths are introduced when $\gamma > 0$ ($\gamma < 0$). From Eq. (6), one finds

$$p_j^{*'} = \frac{\sum_i s_i^\gamma A_{ij} s_j^\gamma}{\sum_{i,j} s_i^\gamma A_{ij} s_j^\gamma}, \qquad (7)$$

which emphasizes that the equilibrium density of walkers at j now depends on the strength of j and of its neighbors for any $\gamma \neq 0$. In the heterogeneous mean-field approximation where the adjacency matrix is factorized $A_{ij} \approx s_i s_j/2W$, one recovers the approximate expression $p_j^{*'} = s_j^{\gamma+1}/(N\langle s_j^{\gamma+1}\rangle)$ [5,9,10].

Another interesting class of BRWs is one where bias is performed toward the high eigenvector centrality node [15–20], $\alpha_i = v_i$, where v is the dominant eigenvector of A [21], namely $\sum_j A_{ij} v_j = \lambda_1 v_i$ and λ_1 is the largest eigenvalue. This bias leads to the maximal-entropy random walk defined by

$$p_{i;t+1} = \sum_j \frac{v_i A_{ij}}{\lambda_1 v_j} p_{j;t}, \qquad (8)$$

which is known to be maximally dispersing on the graph [16], in the sense that the entropy rate is optimal. By defining a flow

graph whose adjacency matrix has the form $A'_{ij} = v_i A_{ij} v_j$, an URW on A' exhibits a stationary probability distribution which is also the solution of Eq. (8), i.e., $p_i^* = v_i^2/Z$, with $Z = \sum_i v_i^2$.

B. Continuous-time random walks

When modeling diffusion, a broad range of processes opens up if walkers can perform their jumps asynchronously. A natural way to implement this situation is to switch from a discrete-time to a continuous-time perspective [22], which finds many applications in biological and physical systems. Passage to continuity can be done in many ways, each leading to a different stochastic process. In the following, we restrict the scope to Markovian processes where the waiting times between two jumps are Poisson distributed. Without loss of generality, we also assume that walkers jump in an unbiased way, while keeping in mind that any BRW can be seen as an unbiased process on the associated flow graph. The time interval between two jumps is determined by the so-called waiting time distribution $\psi(i;t) = r_i e^{-r_i t}$. The rate r_i at which walkers jump may, in general, be nonidentical and depends on the node i where the walker is located. Different sets of $\{r_i\}$ generate different stochastic processes, though the sequence of nodes visited $i_0, i_1, \ldots, i_\tau$, where i_τ is the node visited after τ jumps does not depend on the $\{r_i\}$. For different choices of $\{r_i\}$, what changes is only the times at which the jumps are performed and the time intervals spent on the nodes.

Such continuous-time random walks are driven by the rate equation

$$\dot{p}_i = \sum_j \left(\frac{A_{ij}}{s_j} r_j - r_i \delta_{ij} \right) p_j \equiv -\sum_j L_{ij} p_j, \quad (9)$$

whose stationary solution $p_i^* = s_i/(Zr_i)$, with $Z = \sum_i s_i/r_i$, can be intuitively understood as the probability of arriving at a node times the characteristic time $\approx 1/r_i$ spent on it. Standard choices for the jumping rates include the uniform rate $r_i = 1$ $\forall i$, and the strength-proportional rate $r_i = s_i$ $\forall i$, for which one recovers the standard forms of the Laplacian operator $L_{ij} = \delta_{ij} - A_{ij}/s_j$ and $L_{ij} = s_i \delta_{ij} - A_{ij}$, respectively [5].

This continuous-time random walk can also be viewed as a discrete-time URW, i.e., $p'_{i;t} = \sum_j T'_{ij} p'_{j;0}$, on a flow graph defined by the adjacency matrix

$$A'_{ij}(t) = (e^{-tL})_{ij} Z p_j^* = (e^{-tL})_{ij} \frac{s_j}{r_j}. \quad (10)$$

The definition [Eq. (10)] follows from the solution of Eq. (9) which gives $p_i(t) = \sum_j (e^{-tL})_{ij} p_j(0)$. In fact, one can interpret the probability distribution of a continuous-time random walk at time t as the result of one step random walk driven by the transition matrix $T'_{ij}(t) = A'_{ij}(t)/s'_j$. As previously, $A'_{ij}(t)$ is the flow of probability from j to i at stationarity. One easily verifies that $A'_{ij}(t)$ is symmetric due to detailed balance, i.e., $\sum_j T'_{ij} p'^*_j = \sum_i T_{ij} p'^*_i$ at equilibrium, and that $\sum_j A'_{ij}(t) = \frac{s_i}{r_i}$ at all times. The associated flow graph naturally summarizes how random walkers probe the network over a certain time scale and provides a representation of the system over this scale [5].

III. CONSENSUS PROCESSES

Another kind of interesting processes belonging to the class [Eq. (1)] is the so-called "distributed consensus," for which nodes imitate their neighbors so as to reach a uniform, coordinated behavior. In its simplest form, consensus dynamics is implemented by the so-called agreement algorithm [23]. Each node i is endowed with a scalar value x_i which evolves as

$$x_{i;t+1} = \frac{1}{s_i} \sum_j A_{ij} x_{j;t}. \quad (11)$$

At each time step, the value on a node is updated by computing a weighted average of the values on its neighbors. If the graph is connected and nonbipartite, consensus is asymptotically achieved and each node reaches the uniform value $x^* = \sum_i x_{i;0} s_i/(2W)$ given by a weighted average of the initial conditions. The agreement algorithm [Eq. (11)] is different from an URW, e.g., it does not conserve $\sum_i x_i$ except if the graph is regular. Nonetheless, it has the interesting property that it is the dual of the URW, as it is driven by the transpose of Eq. (3) [3,24]. Moreover, both processes can be seen as two interchangeable facets of the same dynamics, as their spectral properties are related by a trivial transformation, namely the left and right eigenvectors of Eq. (3) are related by $v^R_{\alpha;i} = s_i v^L_{\alpha;i}$, where $\alpha \in [1, N]$ is an index over the eigenvectors.

Similarly to the URW, Eq. (11) can be generalized either by introducing a bias in the weighted average or by tuning the rate at which nodes compute the average of their neighbors' values. The broad class of consensus dynamics generated by this scheme includes, for instance, models from opinion dynamics [24] and a linearized approach to synchronization of different variants of the Kuramoto model [25–28]. However, what is most important is that, for any bias, the duality to the random walk [Eq. (2)] allows us to introduce a consensus process as Eq. (11) on the associated flow graph, analogous to Eq. (5).

IV. DISCUSSION

The behavior of complex systems is determined by their structure and their dynamics [3]. A purely structural analysis, where properties of the adjacency matrix are considered without any insight on underlying dynamical processes, provides only a partial understanding of the system. Here, we have focused on a broad range of linear processes on networks. Some examples where this kind of processes is used is for modeling diffusion or synchronization, and they all exhibit distinct dynamical properties. These properties are summarized by their associated flow graph $\mathcal{G}'$, where the weight of a link is dictated by the patterns of dynamical flow at equilibrium. The definition of $\mathcal{G}'$ has the advantage of simultaneously representing the network topology and its dynamics, and of properly emphasizing nodes and edges, which are important from a dynamical point of view. As shown in Fig. 1, details of the underlying dynamics strongly affect the importance of nodes and their associated ranking [18]. Standard network metrics can be measured on the flow graph in order to uncover other aspects of its dynamical organization [29], for instance, to measure centrality for BRWs [11].

An important context where our formalism proves useful is community detection [13]. The modular structure of a network is often uncovered by optimizing a quality function for the partition $\mathcal{P}$ of the nodes into communities [30]. The widely used modularity [31] measures if links are more abundant within communities than would be expected on the basis of chance. Because of its combinatorial nature, modularity is known to be insensitive to important structural properties which may constrain a flow taking place on the network [4]. Alternative quality functions have thus been developed based on the idea that a flow of probability should be trapped for long times in communities when the partition is good [4–6]. An interesting quantity is the so-called stability $R(t)$ [6] which is defined as the probability for a random walker to be in the same community initially and at time t, when the system is at stationarity. Stability is, in general, different from modularity, but they coincide when the random walk is discrete time and unbiased, the network undirected, and $t = 1$. The notion of a flow graph naturally reconciles combinatorial and flow-based approaches, as the stability of a graph for any process is equal to the modularity of its corresponding flow graph [5], and allows for the detection of modules adapted to the system under scrutiny. In systems where dynamical processes are known to differ from URWs, the notion of a flow graph thus provides the means to apply standard combinatorial methods while still properly taking into account the dynamical importance of nodes and links.

The equivalence between trajectories of a biased (or continuous-time) random walker on $\mathcal{G}$ and those of an URW on $\mathcal{G}'$ also has important practical implications, as it allows us to make use of well-known theoretical results to improve our understanding of BRW processes. For instance, the conditions for convergence and asymptotic stationary solutions for BRW can be obtained through intuitive arguments thanks to the concept of flow graphs, as well as exact expressions for the mean first-passage time [32,33] or spectral properties [34]. This theoretical framework might prove useful to address several problems related to BRWs, such as the search of local biases α_i optimizing in some way the performance of the system [20], for instance, by balancing load on the nodes and improving search in routing systems [11,35], or enhancing the prediction of missing links in empirical data sets [36].

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