PHYSICAL REVIEW E **78**, 065102(R) (2008)

Entropy rate of diffusion processes on complex networks

Jesús Gómez-Gardeñes[1,2,*] and Vito Latora[3]
[1]Scuola Superiore di Catania, Via S. Nullo 5/i, 95123 Catania, Italy
[2]Institute for Biocomputation and Physics of Complex Systems (BIFI), University of Zaragoza, Zaragoza 50009, Spain
[3]Dipartimento di Fisica e Astronomia, Università di Catania and INFN, Via S. Sofia 64, 95123 Catania, Italy

(Received 15 December 2007; revised manuscript received 25 July 2008; published 11 December 2008)

We introduce the concept of entropy rate to characterize a diffusion process on a complex network. The entropy rate represents the minimal amount of information necessary to describe the diffusion on the network, and is a quantity extremely sensitive to the network topology and dynamics. By opportunely tuning the kind of diffusion, the entropy rate allows one to extract different properties of the network structure. Moreover, entropy maximization indicates how to design optimal diffusion processes, providing a new theoretical tool with applications to social, technological, and communication systems.

DOI: 10.1103/PhysRevE.78.065102 PACS number(s): 89.75.Hc, 02.50.Ga, 89.75.Fb

Entropy is a key concept in statistical thermodynamics [1], in the theory of dynamical systems [2], and in information theory [3]. In the realm of complex networks [4,5], the entropy has been used as a measure to characterize properties of the topology, such as the *degree distribution* of a graph [6], or the *shortest paths* between couples of nodes, with the main interest in quantifying the information associated with locating specific addresses [7], or to send signals in the network [8]. Alternatively, various authors have studied the entropy associated with *ensembles of graphs*, and provided, via the application of the maximum entropy principle, the best prediction of network properties subject to the constraints imposed by a given set of observations [9–11].

The main theoretical and empirical interest in the study of complex networks is in understanding the relations between structure and function. Many of the interaction dynamics taking place in social, biological, and technological systems can be analyzed in terms of *diffusion processes* on top of complex networks, e.g., data search and routing, information, and disease spreading [4,5]. It is therefore of utmost importance to relate the properties of a diffusion process with the structure of the underlying network [12,13].

In this paper, we show how to associate an *entropy rate* to a diffusion process on a graph. In this context, the entropy rate is a quantity more similar to the Kolmogorov-Sinai entropy rate of a dynamical system [2,14] than to the entropy of a statistical ensemble [1,4], and measures what is, on average, the shortest per step description of the diffusion on the network [3]. Therefore a high entropy rate indicates a large randomness, or easiness of propagating from one node to another, and can be related to an efficient spreading over the network [14]. Differently from the network entropies previously defined, the entropy rate of a diffusion depends both on the dynamical process and on the graph topology. This allows us to use the entropy rate in two different ways: (i) to characterize with a single measure various structural properties of real-world networks, and (ii) to design optimal diffusion processes which maximize the entropy. As an example of the powerful possibilities of the introduced measure, we consider the diffusion of random walkers whose motion is biased accordingly to a generic topogical or dynamical node property. In particular, for degree-biased random walks we find (i) the analytical expression for the entropy rate in scale-free networks, as a function of the bias; (ii) the dependence of the entropy on the degree distributions and correlations; (iii) the optimal bias which maximizes the entropy in different real networks.

Let us consider a connected undirected graph with N nodes and K links, described by the adjacency matrix $A=\{a_{ij}\}$, and a diffusion process that can be represented as a time invariant *ergodic Markov chain* with a transition matrix $\Pi\equiv(\pi_{ji})$ [3]. The entry π_{ji} is the probability to go, in one time step, from node i to node j, and satisfies the normalization $\Sigma_j\pi_{ji}=1\,\forall\, i$. If the N-dimensional column vector $\mathbf{w}(t)=[w_1(t),w_2(t)\cdots w_N(t)]^{\top}$ represents the node occupation probabilities at time t [with $\Sigma_{i=1}^{N}w_i(t)=1\,\forall\, t$], then the dynamical evolution of the diffusion process can be expressed as $\mathbf{w}(t+1)=\Pi\mathbf{w}(t)$. An ergodic Markov chain has a unique *stationary distribution* $\mathbf{w}^*$, such that $\lim_{t\to\infty}\Pi^t\mathbf{w}(0)=\mathbf{w}^*$ for any initial distribution $\mathbf{w}(0)$. The dynamical properties of the diffusion over the graph can be accounted by evaluating the *entropy rate* of the associated Markov chain that, in the case of an ergodic Markov chain, is given by [3]

$$h=-\sum_{i,j}\pi_{ji}\times w_i^*\ln(\pi_{ji}), \qquad (1)$$

where w_i^* is the i component of the stationary distribution. The value of h measures how the entropy of the process grows with the number of steps. In the information-theoretic language, the entropy rate h is the minimal amount of information necessary to describe the diffusion process on the graph. To evaluate h for a given graph we need to calculate $\mathbf{w}^*$. This can be done analytically for a general class of diffusion processes such as random walks in which, at each time step, the walker at node i chooses one of the first neighbors of i, let say j, with a probability $f_j\equiv f(x_j)$ depending on the node property x_j. The node property x can be topological (degree, betweenness, clustering coefficient, etc.) or any other quantity relevant to the diffusion dynamics (node congestion, healthy state, etc) [5]. In the case of an undirected

*Corresponding author: jesus.gardenes@ct.infn.it

and connected network, such random walks are described by an ergodic Markov chain [15] with a transition probability matrix Π:

$$\pi_{ji} = \frac{a_{ij} f_j}{\Sigma_j a_{ij} f_j}. \quad (2)$$

To calculate $\mathbf{w}^*$ we consider the probability $W_{i\to j}(t)$ of going from node i to node j in t time steps,

$$W_{i\to j}(t) = \sum_{j_1, j_2, \ldots, j_{t-1}} \pi_{i,j_1} \times \pi_{j_1,j_2} \times \cdots \times \pi_{j_{t-1},j}. \quad (3)$$

Since the network is undirected we have $a_{ij}=a_{ji} \forall i,j$. Hence the relation between the two probabilities $W_{i\to j}(t)$ and $W_{j\to i}(t)$ can be written as

$$c_i f_i W_{i\to j}(t) = c_j f_j W_{j\to i}(t), \quad (4)$$

where $c_i = \Sigma_j a_{ij} f_j$. The above relation implies that for the stationary distribution $\mathbf{w}^*$ the equation $c_i f_i w_j^* = c_j f_j w_i^*$ holds, and hence $\mathbf{w}^*$ reads

$$w_i^* = \frac{c_i f_i}{\Sigma_l c_l f_l}. \quad (5)$$

By plugging expressions (2) and (5) into the definition of entropy (1), we finally get a closed form for the entropy rate of a diffusion process on the graph.

As an example of the potential of the introduced entropy rate, we consider the case in which f_j has a power law dependence: $f_j = x_j^\alpha$ with $\alpha \in \mathbb{R}$. In this way, by changing the exponent α we can tune the dependence of the diffusion process on the node property x, and we can visit the graph in various ways. When $\alpha \neq 0$ we are introducing in the random movement of the particle a bias towards high-x ($\alpha > 0$) or low-x (when $\alpha < 0$) neighbors. On the other hand, when $\alpha = 0$ the standard (unbiased) random walk is recovered. The entropy rate reads

$$h = \frac{\Sigma_i x_i^\alpha \Sigma_j a_{ij} x_j^\alpha \ln(x_j^\alpha) - \Sigma_i x_i^\alpha c_i \ln(c_i)}{\Sigma_i c_i x_i^\alpha} \quad (6)$$

and, as expected, it depends on the the kind of bias in the random walker and also on the graph topology.

Our focus now is to investigate the entropy rate of biased random walks in real and synthetic scale-free (SF) graphs with a power-law degree distribution $P_k \sim k^{-\gamma}$, and $\gamma > 2$ [4,5]. A natural choice in such a case is to consider *degree-biased* random walks, i.e., to take $x_j = k_j$.

Synthetic SF networks. Let us start with the particular case $\alpha=0$ where the transition probability reads $\pi_{ji} = a_{ij}/k_i$, and the stationary distribution is $w_i^* = \frac{k_i}{2K}$. Substituting this expression in Eq. (1) and changing the sum over node indexes into a sum over degree classes, we can write the entropy rate of an unbiased walk on a network with degree distribution P_k as

$$h = \frac{N}{2K} \sum_k k P_k \ln(k) = \frac{\langle k \ln(k) \rangle}{\langle k \rangle}. \quad (7)$$

In the case of SF networks of size N, the value of h can be easily expressed as a function of γ and N taking into account that the maximum degree of the network is $k_{max} \sim k_0 N^{1/(\gamma-1)}$,

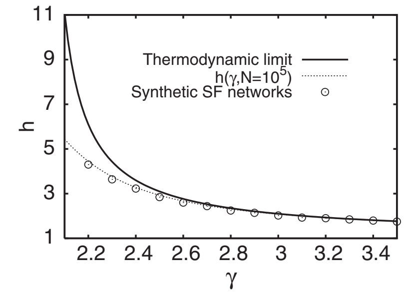

FIG. 1. Entropy rate h of unbiased random walks on SF networks with $N=10^5$ nodes as a function of the exponent γ of the degree distribution. Numerical results (circles) are compared with the two analytical curves corresponding to Eq. (8) (dashed line) and to the limit $N \to \infty$ (solid line).

with k_0 being the minimum degree of a node. From Eq. (7), and approximating k as a continuum variable, we get

$$h(\gamma, N) = \ln(k_0) + \frac{1}{\gamma - 2} + \frac{N^{(2-\gamma)/(\gamma-1)} \ln(N)}{(\gamma - 1)(N^{(2-\gamma)/(\gamma-1)} - 1)}. \quad (8)$$

The above expression diverges for SF networks when $\gamma \to 2$. Conversely, when $\gamma > 2$ SF networks have a finite entropy in the thermodynamic limit $N \to \infty$: $h(\gamma) = \ln(k_0) + \frac{1}{\gamma-2}$.

In order to check the analytical results we have constructed ensembles of 10^2 SF networks with $N=10^5$ nodes and different values of γ. We have obtained numerically the stationary distribution $\mathbf{w}^*$, and computed the entropy directly from Eq. (1). The results, averaged over the ensemble of networks, are reported in Fig. 1 as a function of γ. We notice a good agreement between numerics and Eq. (8).

Let us now concentrate on the general case $\alpha \neq 0$. The entropy rate of Eq. (6) can be rewritten by changing again the sums over node indexes into sums over degree classes, as

$$h = -\frac{\Sigma_k k^\alpha P_k [C_k \ln(C_k) - \alpha k \Sigma_{k'} k'^\alpha P_{k'|k} \ln(k')]}{\Sigma_k C_k k^\alpha P_k}, \quad (9)$$

where $C_k = k \Sigma_{k'} k'^\alpha P_{k'|k}$, and $P_{k'|k}$ is the conditional probability that a link from a node of degree k ends in a node with degree k'. We notice that the entropy rate of degree-biased random walks depends on the degree distribution of the network P_k and on the conditional probabilities $P_{k'|k}$. In the particular case of a network with no degree-degree correlations we can write $P_{k'|k} = k' P_{k'} / \langle k \rangle$, and the expression for the entropy reduces to

$$h = (1 - \alpha) \frac{\langle k^{\alpha+1} \ln(k) \rangle}{\langle k^{\alpha+1} \rangle} + \ln\left(\frac{\langle k^{\alpha+1} \rangle}{\langle k \rangle} \right). \quad (10)$$

This expression only depends on the degree distribution of the network. For SF networks, we get in the the continuum-degree approximation:

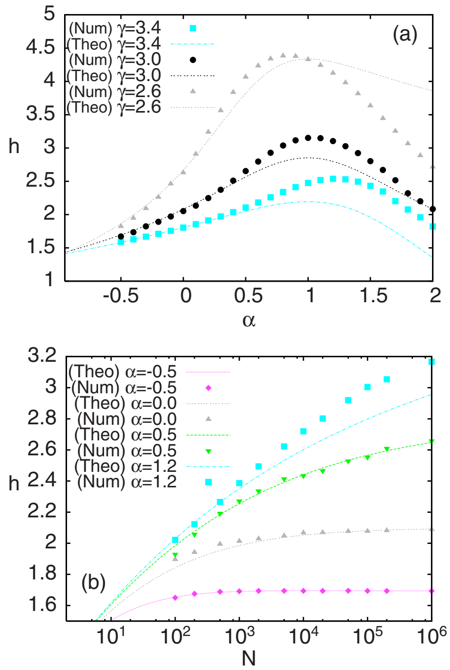

FIG. 2. (Color online) (a) Entropy rate h, as a function of α, for α-biased random walks on SF networks with $N=10^5$ nodes and $\gamma=2.6,3,3.4$. Symbols represent the values of h found numerically, while the lines are the corresponding analytical predictions $h(\gamma,\alpha,N)$ of Eq. (11). (b) Entropy rate h for α-biased random walks on SF networks with $\gamma=3$, as a function of the system size N and for several values of α. Again, symbols are the results of numerical simulations, while the lines correspond to Eq. (11).

$$h(\gamma,\alpha,N)=\frac{1-\alpha}{\gamma-\alpha-2}+\frac{(1-\alpha)N^{(\alpha+2-\gamma)/(\gamma-1)}\ln(N)}{(\gamma-1)(N^{(\alpha+2-\gamma)/(\gamma-1)}-1)}+\ln\left[\frac{k_0(\gamma-2)(N^{(\alpha+2-\gamma)/(\gamma-1)}-1)}{(\gamma-\alpha-2)(N^{(2-\gamma)/(\gamma-1)}-1)}\right]. \quad (11)$$

When $N\to\infty$, the entropy rate in SF networks with $\gamma<2+\alpha$ diverges as $h\sim\ln(N)$. On the other hand, when $\gamma>2+\alpha$, the entropy rate in the limit $N\to\infty$ is finite and equal to

$$h(\gamma,\alpha)=\frac{1-\alpha}{\gamma-\alpha-2}+\ln\left[\frac{k_0(\gamma-2)}{\gamma-\alpha-2}\right]. \quad (12)$$

Such an expression, valid in infinite size limit, shows a monotonic growth of the entropy $h(\gamma,\alpha)$ with the degree-bias α, with h tending to infinity as $\alpha\to(\gamma-2)^-$. More interestingly, the entropy rate in finite networks, Eq. (11), shows a single maximum at a value of α that depends on γ. This result indicates that, for a given network, it is possible to maximize the entropy of the process by opportunely tuning the bias α of the walker.

To check the above analytical expressions we have computed numerically the entropy rate of degree-biased random walkers on computer-generated uncorrelated SF networks, as we did for the unbiased case. In Fig. 2(a) we report the entropy rate as a function of the degree bias α for SF networks of size $N=10^5$. In Fig. 2(b) we show the scaling of h with the system size N, in SF network with $\gamma=3$. In both

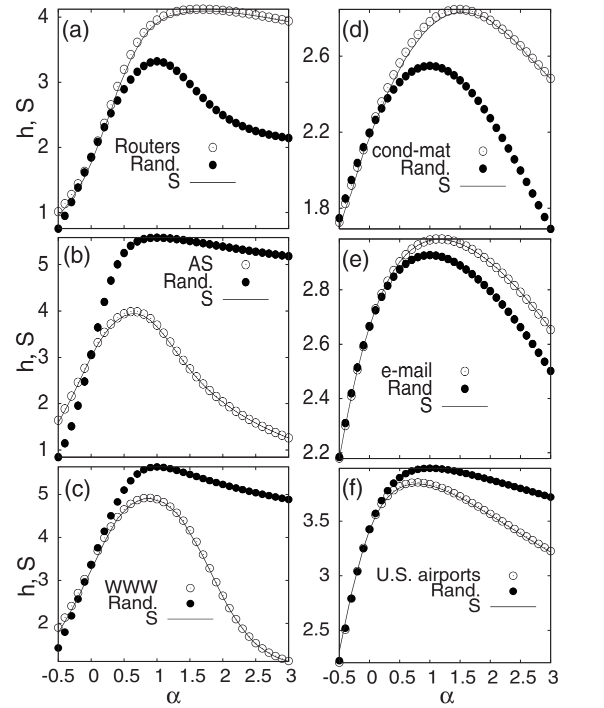

FIG. 3. Entropy rate h for α-biased random walks on six real networks (filled circles). The networks from (a) to (f) correspond to Refs. [18–22]. In each case, h is compared to the entropy rate h^{Rand} obtained on a randomized version of the network (full circles). The continuous line is the numerical computation of the entropy S [Eq. (13)]. The three measures are shown as a function of α.

cases Eq. (11) is in good agreement with the numerical results reproducing the qualitative behavior of h as a function of α (being the global maximum of h well reproduced) and N (being both the divergence of h, for $\alpha>\gamma-2$, and the asymptotic finite value of h, when $\alpha<\gamma-2$, correctly reproduced)

Real SF networks. Up to now, we focused on the entropy rate of biased random walks on SF networks. However, real networks are not perfect scale free and show additional topological properties such as degree-degree correlations, structural motifs, nonvanishing clustering coefficient, etc., [4,5]. Therefore one important question regarding real networks is to unveil how a diffusion process is affected by these topological features. To this end, we compare the entropy rate for a real network with the value h^{Rand}, obtained from Eq. (10), for a randomized network with the same degree sequence and no correlations [16]. In Fig. 3 we report the entropies h and h^{Rand} as a function of the bias parameter α for six real networks. We find that the entropy of real networks h is either larger or smaller than h^{rand} for all the range of positive values of α [17]. We have observed the same behavior in other real communication, technological, and social networks analyzed. Our experiments reveal that social networks have always $h>h^{Rand}$, while the other networks have $h<h^{Rand}$, with the exception of Internet routers. This difference in the entropy rate has its roots on the nature of degree-degree correlations, and points out that assortativity plays a key role in facilitating the spread of information across the whole network.

More interestingly, all the real networks studied present a well defined maximum for the entropy rate at some finite value α^{opt} of the bias parameter. Therefore a byproduct of the analysis presented here is the possibility to design optimal diffusion processes by finding the value α^{opt} where the entropy rate is maximal. In particular, our results for degree biased random walks indicate that, for assortative networks (e.g., social networks), the maximal entropy rate is obtained with a value $\alpha^{opt}>1$ while, for disassortative networks, α^{opt} is located in the sublinear bias region.

Optimal diffusion processes. What are the interesting features of a diffusion process with maximal entropy rate? To illustrate the physical meaning of h and α^{opt} in a practical case, let us consider a communication network in which, under stationary conditions, a large number of M information packets are sent from node to node according to a degree-biased rule. The goal of each node is to spread information about its current state (such as its healthy or infected state, its availability to perform tasks, etc.) to other nodes in the most efficient way. The state of a given node can be represented by assigning to each node a different *color* c $(c=1,\ldots,N)$. For instance, we color node i, and also all $n_i \propto w_i^*$ packets located at node i at time t, with color $c_i=i$. After this coloring, the n_i packets are delivered to the neighbors of i, thus passing the color (the information about the state i at time t) to them. All the nodes make the deliveries simultaneously, and after the exchange process every node i contains packets of different colors. The most efficient routing policy is such that the entropy S of the distribution of colors across the nodes of the network, after the diffusion step, is maximal. This entropy can be written as

$$S=\sum_{i=1}^{N}\frac{n_i}{M}S_i \quad \text{with } S_i=-\sum_{c=1}^{N}\frac{n_i^c}{n_i}\ln\frac{n_i^c}{n_i}, \tag{13}$$

where S_i is the entropy of the color distribution at node i, and n_i^c $(\sum_{c=1}^{N}n_i^c=n_i \forall i)$ is the number of packets of color c at node i. Hence S is the node average of S_i, weighted by the number of packets that a node is handling. Since n_i^c is equal to the number of packets arrived to i from node $j=c$, by simple algebra it is easy to prove that $S=h$. We have confirmed numerically that the average entropy of the color distribution per node is equal to the entropy rate, by performing simulations of the color exchange dynamics on top of the six real networks. In Fig. 3, the values of S are reported as a function of α. In conclusion, the bias α^{opt} for which the entropy rate h is maximal corresponds also to the maximal entropy S of the color distribution. Therefore finding the diffusion process with maximal entropy rate for a given network topology is equivalent to designing the routing policy for which the average information of network elements about the status of their neighbors at the previous time step is maximal.

Summing up, in this paper, we have introduced the entropy rate of a diffusion process, a measure that is particularly suited to capture the interplay between network structure and diffusion dynamics. We have studied how the entropy rate of degree-biased random walks depends on the topology of synthetic and real networks. Our results indicate that it is possible to tune a diffusion process in order to maximize its entropy rate on a given topology. This maximization allows us to obtain systems where the information of nodes about the state of the rest of the network elements is maximal. Therefore the concept of entropy rate and its maximization can find useful applications to information dissemination in social networks, transfer of data in grid computing systems, or to the design of efficient vaccination campaigns. The approach adopted here can be easily extended to more general network topologies, such as weighted graphs and also, with some appropriate modifications, to directed and unconnected graphs.

We are indebted to M. Chavez and H. Touchette, and to two anonymous referees for their valuable comments. This work was supported by the Engineering and Physical Sciences Research Council (Grant No. EP/F013442/1).

[1] R. Balian, *From Microphysics to Macrophysics* (Springer-Verlag, New York, 1991).
[2] C. Beck and F. Schlögl, *Thermodynamics of Chaotic Systems* (Cambridge University Press, Cambridge, England, 1993).
[3] T. M. Cover and J. A. Thomas, *Elements of Information Theory* (Wiley, New York, 1991).
[4] M. E. J. Newman, SIAM Rev. **45**, 167 (2003).
[5] S. Boccaletti, V. Latora, Y. Moreno, M. Chavez, and D.-U. Hwang, Phys. Rep. **424**, 175 (2006).
[6] R. Ferrer, I. Cancho, and R. V. Solé, Lect. Notes Phys. **625**, 114 (2003).
[7] M. Rosvall, A. Trusina, P. Minnhagen, and K. Sneppen, Phys. Rev. Lett. **94**, 028701 (2005).
[8] A. Trusina, M. Rosvall, and K. Sneppen, Phys. Rev. Lett. **94**, 238701 (2005).
[9] G. Bianconi, Europhys. Lett. **81**, 28005 (2008).
[10] P. Minnhagen and S. Bernhardsson, Chaos **17**, 026117 (2007).
[11] J. Park and M. E. J. Newman, Phys. Rev. E **70**, 066117 (2004).
[12] L. da Fontoura Costa *et al.*, Appl. Phys. Lett. **91**, 054107 (2007).
[13] M. Rosvall and C. T. Bergstrom, Proc. Natl. Acad. Sci. U.S.A. **105**, 1118 (2008).
[14] V. Latora and M. Baranger, Phys. Rev. Lett. **82**, 520 (1999).
[15] F. R. Gantmacher, *The Theory of Matrices*, (Chelsea Publishing Company, New York, 1959) Vol. 2.
[16] S. Maslov and K. Sneppen, Science **296**, 910 (2002).
[17] For $\alpha=0$ both the real network and the randomized ensemble have the same value of h, since in this limit Eq. (10) is exact and only depends on the degree sequence.
[18] A. Vázquez, R. Pastor-Satorras, and A. Vespignani, Lect. Notes Phys. **650**, 425 (2004).
[19] R. Albert, H. Jeong, and A. L. Barabási, Nature (London) **401**, 130 (1999).
[20] M. E. J. Newman, Phys. Rev. E **64**, 016131 (2001).
[21] R. Guimera, L. Danon, A. Díaz-Guilera, F. Giralt, and A. Arenas, Phys. Rev. E **68**, 065103(R) (2003).
[22] V. Colizza, R. Pastor-Satorras, and A. Vespignani, Nat. Phys. **3**, 276 (2007).