DYNAMICAL PROPERTIES OF DIFFUSION PROCESS ON COMPLEX NETWORKS WITH ARBITRARY DEGREE DISTRIBUTION

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Dynamical properties of diffusion process on complex networks with arbitrary degree distribution are investigated. The rule of the diffusion process encompasses both the structural characteristics and the information processing dynamics. Considering the influence of a node on the global dynamical behavior, the dynamical generating function of the process, which is deeply reflecting the basic characteristic of the process and mutually decided with the dynamical process, is proposed. Based on the analysis of the dynamical generating function we introduce dynamical centrality for each node, which determines the relative importance of nodes and the capability of the given node to collect and communicate information with its neighbouring environment in the network via the diffusion process. Furthermore, a new parameter, dynamical entropy, is proposed to measure the interplay between dynamical centrality and diffusion dynamics. The experimental results on large-scale complex networks with Poisson distribution confirm our analytical prediction.

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1. Introduction

In the past decades, various topological and dynamical properties of networks resulting from real systems have attracted many researchers in diverse fields [1–5]. The inherent complexity of networks results in rich behaviors in the dynamical processes of the physical systems depending on the topological structure of networks. For example, random walk [5–8], in addition to biased random walk [9], has been widely investigated to understand the

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essential dynamical properties of physical systems on networks [10–12] and also has many practical applications to real networks such as information searching in the Internet, and so on [13–16].

Based on the random walk on complex networks, evaluation of the importance of nodes and edges is widely used in analysis of complex networks. To evaluate the importance, various centrality measures, *e.g.*, degree centrality, closeness centrality, and betweenness centrality, have been proposed [17–19]. For example, betweenness centrality (BC) [20] is introduced as a good approximation for the quantity of information passing through a node in communication networks [21,22]. However, BC is just relying on the shortest paths that is the unbiased dynamical process with treating the neighbors equally.

In the informational sense, the entropy is a measure of the uncertainty about dynamical behaviors of the network. In a network with higher entropy, more information is needed to describe its future behavior, and its effective complexity is higher [23,24]. In the field of complex networks, entropy has been applied to characterize the topological properties, such as the degree distribution [25], the shortest paths between couples of nodes [26], and even more the dynamical processes on complex networks [27]. Recently, the entropy rate of a diffusion process was introduced in Ref. [28] to characterize a diffusion process. Combining the maximum entropy principle, it is possible to design optimal diffusion processes. Furthermore, in Ref. [29], a new class of random walk processes was introduced, the maximal entropy random walk (MERW), which induced a surprising effect of localization in the presence of weak disorder. Alternatively, many results on entropy are associated with the structure of the network, or the information flow on the network respectively. They are rarely functions comprehending the structure and the information flow on the network.

The main theoretical and empirical problem in the study of complex networks is how to construct a function which can closely incorporate the structure of the network and the dynamical process on it. Many interaction dynamics in social, biological and technological systems can be analyzed in terms of diffusion processes on complex networks, *e.g.*, information diffusion and disease spreading [30,31]. It is, therefore, utmost important to relate the properties of a diffusion process with network structure and the information flow on it.

In this paper, we investigate the dynamical properties of the diffusion process on complex networks. The structure of this paper is as follows. In Section 2, we review the diffusion process on complex networks, in which the rule of the diffusion process comprehends both the structural characteristics and the information flow. In Section 3, we discuss the dynamical generating function for diffusion process, which can be mutually decided with the dynamical process. For special cases, the dynamical generating function is evolved to the generating function of the topological structure and the information function of the dynamical process. In Section 4, the dynamical centrality, which exhibits the capability of a node collecting and communicating information with its neighbor environment over the network in the diffusion process is proposed. Furthermore, to measure the interplay between dynamical centrality and diffusion process, a new parameter, dynamical entropy, is deeply investigated and the experimental results on large-scale complex networks with Poisson distribution are given. In Section 5, the conclusion is given and the prospect is deeply discussed.

2. Diffusion process on complex networks

We consider a connected undirected graph G with nodes $\{1, 2, \cdots, N\}$ and m links, described by the adjacency matrix $A = (a_{ij})_{N\times N}$ and degree sequence $\{k_1, \cdots, k_N\}$ which satisfies $k_i = \sum_j a_{ij}$ and $\sum_i k_i = 2m$.

Consider a packet as a random walker that hops at discrete time series: a packet at node i and time t will choose one of its neighbors j to hop to with some probability p_{ij}. Here, take

$$p_{ij} = \frac{a_{ij}k_j^{\alpha}}{\sum\limits_{j=1}^{N} a_{ij}k_j^{\alpha}}\,, \tag{1}$$

where α is the adjustment parameter between the global structure and the degree of a node [9]. If the random walker deals with the neighbor nodes indiscriminately, that is, it does not consider the properties of the neighbors, but the connectedness of the graph, we take $\alpha = 0$. But if the walker is predisposed to the degree of the nodes, we take $\alpha > 0$ ($\alpha < 0$) for the trend to the high (low) degree nodes.

We denote $P = (p_{ij})_{N\times N}$ as the probability transition matrix. Supposing the packet starts at node i_0 at time $t = 0$, we define $f_{i_0 j}(t)$ as the probability that the packet stays at node j and time t with the initial state i_0. Then the master equation [6] for the probability $f_{i_0 j}(t)$ is

$$f_{i_0 j}(t+1) = \sum_{l=1}^{N} p_{lj}\, f_{i_0 l}(t)\,. \tag{2}$$

Let $f(t) = (f_1(t), f_2(t), \cdots, f_N(t))$, where $f_j(t) = f_{i_0 j}(t)$ is the probability that the random walker locates at node j at time t, we obtain that $f(t+1) = Pf(t)$. Denote $f_j^{\infty} = \lim_{t\to\infty} f_{i_0 j}(t)$, which is the probability that the random walker stays at node j in the stationary state. By Parron–Frobenius theorem, f_j^{∞} uniquely exists and has no correlation with the initial position of the random walker [32].

As the adjacency matrix of undirected graph is symmetric, if there is a path from i to j represented as $(i, j_1, j_2, \cdots, j_{t-1}, j)$, there must be the corresponding path from j to i $(j, j_{t-1}, \cdots, j_2, j_1, i)$. Then

$$f_{ij}(t) = \sum_{j_1, j_2, \cdots, j_{t-1}} \frac{k_{j_1}^{\alpha}}{\sum_l a_{il} k_l^{\alpha}} \cdots \frac{k_j^{\alpha}}{\sum_l a_{j_{t-1}l} k_l^{\alpha}}\,, \tag{3}$$

and

$$f_{ji}(t) = \sum_{j_1, j_2, \cdots, j_{t-1}} \frac{k_{j_{t-1}}^{\alpha}}{\sum_l a_{jl} k_l^{\alpha}} \cdots \frac{k_i^{\alpha}}{\sum_l a_{j_1 l} k_l^{\alpha}}\,. \tag{4}$$

Denoting $d_i(\alpha) = \sum_l a_{il} k_l^{\alpha}$, we get

$$d_i(\alpha) k_i^{\alpha} f_{ij}(t) = d_j(\alpha) k_j^{\alpha} f_{ji}(t)\,.$$

Let $t \to \infty$, then

$$d_i(\alpha) k_i^{\alpha} f_j^{\infty} = d_j(\alpha) k_j^{\alpha} f_i^{\infty}\,.$$

Hence

$$f_i^{\infty} = \frac{d_i(\alpha) k_i^{\alpha}}{\sum_i d_i(\alpha) k_i^{\alpha}}\,. \tag{5}$$

By equation (5), we can calculate the probability that the random walker stays at node i in the stationary state. Especially, when $\alpha = 0$, $d_i(0) = \sum_j a_{ij} = k_i$, it is just the stationary distribution of the unbiased random walk [6]

$$f_i^{\infty} = \frac{k_i}{\sum_i k_i} = \frac{k_i}{2m}\,, \tag{6}$$

which shows that the biased random walk is popularization of unbiased random walk on complex networks.

3. Dynamical generating function of diffusion process

The main theoretical and empirical interest in the study of complex networks is how to construct a function which can closely comprehend the structure of the network and the dynamical process on it. As the dynamical process of the physical systems depending on the structure of the underling networks can be expressed by the diffusion process, we can analyze the properties of diffusion process to comprehend the dynamical process. The *dynamical generating function* $F(x,t)$ of the diffusion process is defined as follows,

$$F(x,t) = \sum_{i=1}^{N} \sum_{k=1}^{\infty} p(k) \left[f_i(t) x\right]^k\,, \tag{7}$$

in which $p(k)$ is the degree distribution of G (we just consider connected undirected networks, then $p(0) = 0$).

Regarding $x \leq 1$, we get

$$\begin{aligned} F(x,t) &= \sum_{i=1}^{N}\sum_{k=1}^{\infty} p(k)\,[f_i(t)x]^k \\ &\leq \sum_{i=1}^{N}\sum_{k=1}^{\infty} p(k) f_i(t)^k \\ &\leq \sum_{i=1}^{N}\sum_{k=1}^{\infty} p(k) f_i(t) = 1\,. \end{aligned} \tag{8}$$

As a consequence, $F(x,t)$ is convergent for all $t \geq 0$ and $x \leq 1$.

Further understanding of the dynamical generating function $F(x,t)$ can be achieved from the following two special cases.

Case 1: Generating function of topology structure

At time $t = 0$, there is only one walker at the initial node i_0 and no walkers at the other nodes, *i.e.*

$$f_j(0) = \begin{cases} 1\,, & \text{for the initial node } i_0\,, \\ 0\,, & j \neq i_0\,. \end{cases}$$

Then

$$F(x,0) = \sum_{k=1}^{\infty} p(k)x^k = G(x) - p(0)\,, \tag{9}$$

and

$$G(x) = \sum_{k=0}^{\infty} p(k)x^k = F(x,0) + p(0)\,, \tag{10}$$

which is exactly the generating function of the degree distribution. For the structure of the underling networks, the mathematics of generating functions can be used to calculate exactly many of the statistical properties of complex networks [4].

Case 2: Information function of random walk

Since the dynamical process can be expressed by the diffusion process, by the dynamical generating function, we define the *information function* for any time t as

$$H(t) = F(1,t) = \sum_{i=1}^{N}\sum_{k=1}^{\infty} p(k) f_i(t)^k = \sum_{i=1}^{N} q_i(t)\,, \tag{11}$$

where $q_i(t) = \sum_{k=1}^{\infty} p(k) f_i(t)^k$. After normalization, replace $q_i(t)$ with

$$h_i(t) = \frac{q_i(t)}{\sum_i q_i(t)} = \frac{\sum\limits_{k=1}^{\infty} p(k) f_i(t)^k}{\sum\limits_{i=1}^{N} \sum\limits_{k=1}^{\infty} p(k) f_i(t)^k} . \tag{12}$$

For node i with degree k, $f_i(t)^k$ reflects the contribution of node i to its neighbors. $q_i(t)$ is the average contribution of node i for different degrees, and $h_i(t)$ is the normalized contribution which can be considered as the *dynamical centrality of vertex* i.

Considering the case $\alpha = 0$ when the random walk is unbiased, the stationary distribution is

$$f_i^{\infty} = \frac{k_i}{2m} .$$

As an application, we analyze the random walk on a random graph, the degree distribution of which is $p(k) = e^{-c} c^k / k!$ with average degree c. If the graph is unconnected, we consider the random walk on each connected component respectively, and then make a normalization over the whole graph. The stationary distribution for a component with m_c edges is $f_{ic}^{\infty} = k_i/(2m_c)$. Normalizing it over the whole graph we get $f_i^{\infty} = f_{ic}^{\infty}(2m_c)/2m = k_i/2m$, and then

$$q_i(\infty) = \sum_{k=1}^{\infty} e^{-c} \frac{c^k}{k!} \left(\frac{k_i}{2m}\right)^k = e^{c\left(\frac{k_i}{2m} - 1\right)} - e^{-c} , \tag{13}$$

$$H(\infty) = \sum_{i=1}^{N} e^{c(k_i/2m - 1)} - N e^{-c} . \tag{14}$$

To get the average degree c at which the information function reaches the maximum value, let

$$\frac{\partial H}{\partial c} = \sum_{i=1}^{N} e^{c\left(\frac{k_i}{2m} - 1\right)} \left(\frac{k_i}{2m} - 1\right) + N e^{c} = 0 , \tag{15}$$

we apply mean field approximation to equation (15), then

$$c = \ln \left(1 + \frac{1}{N-1}\right)^{N} . \tag{16}$$

From equation (16), we obtain that, the information function achieves the maximum value at $c = 1$ when $N \to \infty$.

For random graphs with $N = 10^3$ but different average degrees, we simulate the information function $H(\infty)$ for different $\alpha = 0,\ 1,\ 2$ and show the corresponding results in Fig. 1 which satisfies our analysis perfectly. It

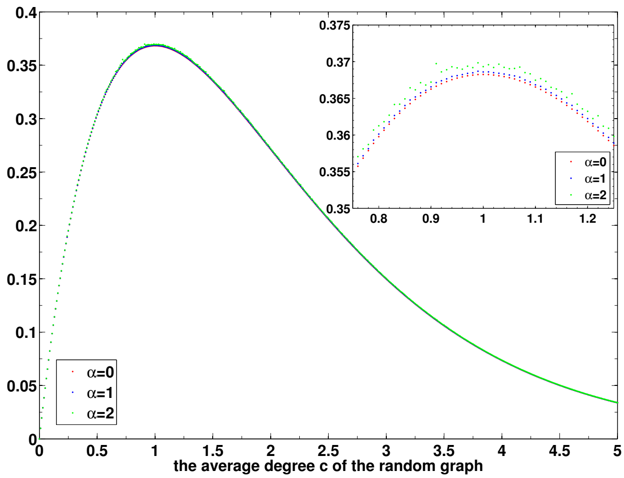

Fig. 1. The information function $H(t)$ when $t \to \infty$ changes with the average degree c of the random graph with $N = 10^3$ when $\alpha = 0,\ 1,\ 2$.

reveals that the giant component appears when the average degree c gets over 1 [33]. Once $c < 1$, the largest component increases quickly along with the increase of the average degree c, and the amount of information received by the random walker also increases. As $c > 1$, the increasing speed of the giant component size slows down[33], and the amount of information received by the random walker continues increasing. However, the increasing rate is lower than that of the time consumed, which induces that the average efficient information $H(\infty)$ decreases along with the increase of c. In the detailed figure in Fig. 1, we can see that the information function increases along with the increase of the adjustment parameter α. We verify it as follows.

For $\alpha \neq 0$,

$$f_i^{\infty} = \frac{d_i(\alpha)k_i^{\alpha}}{\sum\limits_i d_i(\alpha)k_i^{\alpha}}\,,$$

the average contribution of node i is

$$q_i(\infty) = \sum_{k=1}^{N} e^{-c}\frac{c^k}{k!}\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum\limits_i d_i(\alpha)k_i^{\alpha}}\right)^k = e^{c\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum\limits_i d_i(\alpha)k_i^{\alpha}}-1\right)} - e^{-c}\,, \quad (17)$$

and the relative information function is

$$H(\infty) = \sum_{i=1}^{N} e^{c\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum_i d_i(\alpha)k_i^{\alpha}} - 1\right)} - Ne^{-c}. \tag{18}$$

When the random walk is unbiased, the diffusion behavior just relates to the structure of the random graph and does not reflect the information flow on it, which makes the total amount of information small. When the parameter α increases, behaviors of the information do not only depend on the structure, but also rely on the information flow, which leads to the value of information increase along with the increase of parameter α. The information function $H(\infty)$ on the random graph for different adjustment parameter α is shown in Fig. 2, which fits our analysis very well.

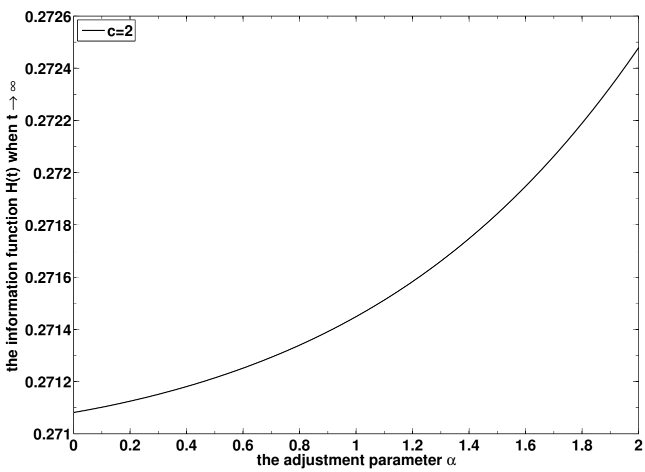

Fig. 2. The information function $H(t)$ when $t \to \infty$ changes with the adjustment parameter α of the random graph with $N = 10^3$ when $c = 2$.

4. The dynamical centrality and entropy

From equation (12), $h_i(t)$ is the normalized contribution which is defined as the *dynamical centrality of vertex i*. Considering the biased random walk on random networks with different α, the dynamical centrality is

$$h_i(\infty) = \frac{e^{c\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum_i d_i(\alpha)k_i^{\alpha}} - 1\right)} - e^{-c}}{\sum_{i=1}^{N} e^{c\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum_i d_i(\alpha)k_i^{\alpha}} - 1\right)} - Ne^{-c}}. \tag{19}$$

In Fig. 3, for $\alpha = -100, -2, 0, 2, 100$, the dynamical centrality h for the nodes with different degrees is shown.

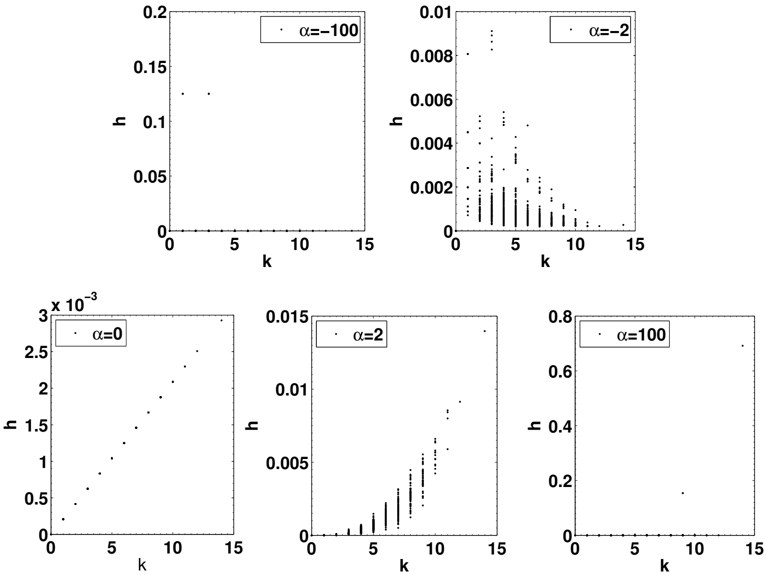

Fig. 3. The dynamical centrality h changes with the degree of node k when $\alpha = -100, -2, 0, 2, 100$.

When $\alpha < 0$, the random walker tends to visit the low degree nodes which have more chance to attract the random walker, and then the dynamical centrality of such nodes is relatively larger than that of the nodes with higher degrees. When $\alpha = 0$, there is no difference between nodes, and the random walker hops to the neighbors with equal probability. The higher the degree, the more important the node, *i.e.*, the dynamical centrality is decided by the degree directly. In contrast to the case of $\alpha < 0$, when $\alpha > 0$ the random walker is attracted by the nodes with high degrees which perfom more importance than those with low degrees. For the extreme cases of $\alpha \to \pm\infty$ represented in Fig. 3 as $\alpha = \pm 100$, the most dynamical important nodes are just focused on very few nodes whose dynamical centrality is nonzero, while others are zero. That is, when $\alpha \to \pm\infty$, these few nodes play the critical role in the dynamical process.

Generally, different cases of α result in different rules of the diffusion process. The stationary distribution depends on not only the degree, but also the information flow. Thus, nodes with the same degree can have different dynamical centrality h which is an exact annotation for the importance of node in the dynamical process. In summary, α can be modulated to distinguish the different important nodes in the dynamical process.

Entropy is a measure of randomness and confusion. To measure the interplay between dynamical centrality and diffusion dynamics, the dynamical properties can be accounted by *dynamical entropy* which is defined as follows:

$$\mathrm{RWE}(t) = -\sum_{i=1}^{N} h_i(t)\ln(h_i(t))\,, \tag{20}$$

where $h_i(t)$ is the dynamical centrality of node i. Since $h_i(t)$ reflects the importance of node i attracting the random walker, $\mathrm{RWE}(t)$ measures the confusion state of the walker at time t.

For different α,

$$h_i(\infty) = \frac{\sum\limits_{k=1}^{\infty} p(k)\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum\limits_i d_i(\alpha)k_i^{\alpha}}\right)^k}{\sum\limits_{i=1}^{N}\sum\limits_{k=1}^{\infty}\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum\limits_i d_i(\alpha)k_i^{\alpha}}\right)^k}\,. \tag{21}$$

For the random graph, we have

$$h_i(\infty) = \frac{e^{c\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum_i d_i(\alpha)k_i^{\alpha}}-1\right)} - e^{-c}}{\sum\limits_{i=1}^{N} e^{c\left(\frac{d_i(\alpha)k_i^{\alpha}}{\sum_i d_i(\alpha)k_i^{\alpha}}-1\right)} - Ne^{-c}}\,. \tag{22}$$

Applying equation (22) into equation (20), experimental results of the dynamical entropy for $\alpha = 0$, 1, 2 and the average trend for RWE along with average degree c are shown in detail in Fig. 4.

As the average degree c increases, the random walker can arrive at more and more nodes, and the final state is more and more jumbled, which induce the increase of the dynamical entropy RWE. As the scale of the giant component increases slowly when $c > 1$ [33], the dynamical entropy RWE performs little increase. According to the Maximum Entropy Principle [34], to investigate dynamical process on the network globally, we can add edges into the network until the giant cluster appears.

In intuition, the RWE decreases along with the increase of α in Fig. 4. To show the detailed difference of the RWE among different adjustment parameter α, numerical verifications are carried out at $c = 3$, 4, 5 and the average trend for RWE along with the adjustment parameter α is described, see Fig. 5.

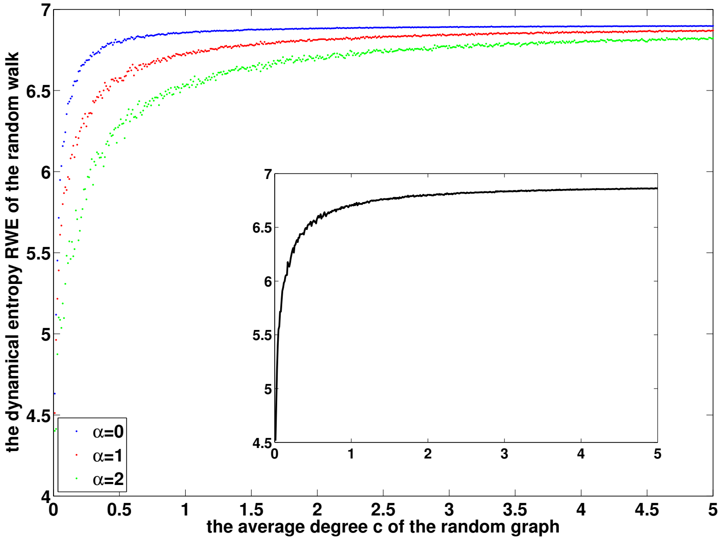

Fig. 4. The dynamical entropy RWE(t) when $t \to \infty$ as a function of the average degree c of the random graph with $N = 10^3$ when $\alpha = 0$, 1, 2 is in the main graph, and the subgraph is the average dynamical entropy as a function of c.

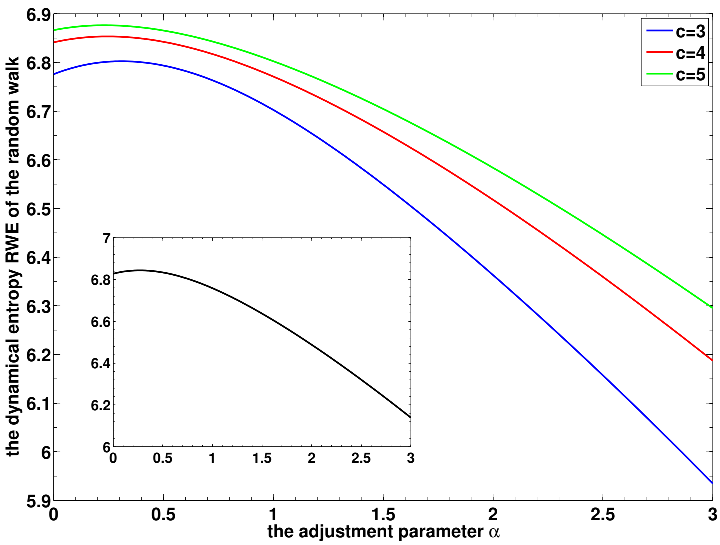

Fig. 5. The dynamical entropy RWE(t) when $t \to \infty$ as a function of the adjustment parameter α of the random walk on random graph with $N = 10^3$ when $c = 3, 4, 5$ is in the main graph, and the subgraph is the average dynamical entropy as a function of α.

When α increases, the random walker is more inclined to access the nodes with high degrees. A little change of degree can lead to enormous change of the attracting ability. Thus, the nodes with large dynamical centrality concentrates on fewer high-degree nodes as α increases, and the walker is more inclined to such more dynamical important nodes, which cause decrease of the level of the confusion and the dynamical entropy RWE decreases, too.

To measure the dynamical centrality on the complex networks, we consider the diffusion process on networks with 1000 nodes and the average degree $c = 5$, and remove either *(i)* the most dynamically important nodes, *(ii)* the nodes with highest degree k_i, *(iii)* random nodes. After removing m nodes, we recalculate the dynamical entropy RWE(m). In Fig. 6, RWE(m)/RWE(0) is shown as a function of m. When $\alpha < 0$, the nodes with low degree contribute more in the dynamical process. In contrary, the nodes with high degree contribute more when $\alpha > 0$, and the degree centrality is just a special situation of the dynamical centrality when $\alpha = 0$, which is reflected in Fig. 6. All these numerical figures show that the dynamical centrality has great influence on the dynamical process on the complex networks.

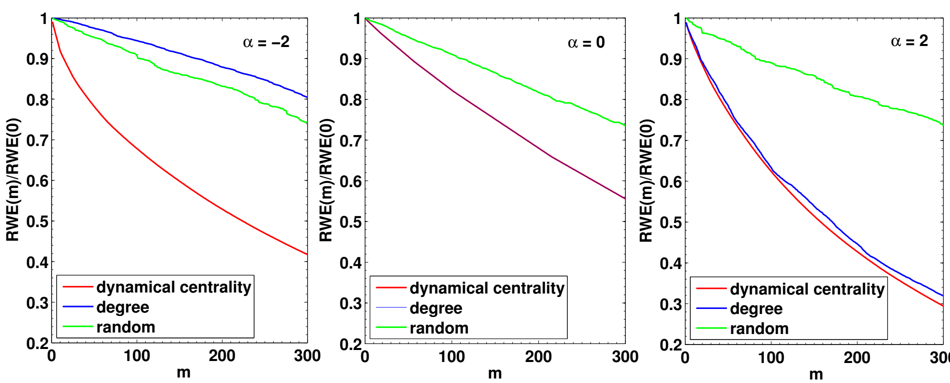

Fig. 6. For different parameter $\alpha = -2, 0, 2$ of random walk, the dynamical entropy changes with the number of vertices taken off, for different cases: by the dynamical centrality, degree, and random.

5. Conclusion

In summary, we have investigated in detail the dynamical properties of the diffusion process on complex networks, in which the rule of the diffusion process comprehends both the structural characteristics and the information flow. Contrast to the generating function of the topological structure, the dynamical generating function for the diffusion process, which is mutually decided with the dynamical process, is introduced and deeply analyzed.

Specially, the dynamical generating function can be evolved to the generating function of the topological structure and the information function of the information flow. For various discussed centrality measures mainly based on unbiased dynamical process with treating the neighbors equally, the dynamical centrality of nodes, exhibiting the capability of a node collecting and communicating information with its neighbor environment over the network in the diffusion process is introduced and employed to evaluate the average contribution of node during the biased process. Furthermore, a new parameter, dynamical entropy, is proposed to measure the interplay between dynamical centrality and diffusion dynamics that can measure the confusion at the stationary state. Experimental results on large-scale complex networks confirm our analytical prediction.

In this paper, the parameter α is considered as a constant all over the process, but in the diffusion process of realistic self-adaptive networks, *e.g.* traffic network and World Wide Web, it has to regulate itself in the diffusion process to optimize the transmission capability over the network. That is, when there are some nodes overloaded, we should modulate α to mitigate the transmission loads to others. In the future work, dynamical self-adaptive parameter $\alpha(t)$ will be considered to realize the network optimization.

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