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Spreading dynamics in heterogeneous graphs: Beyond the assortativity coefficient

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HIGHLIGHTS

- A new kind of random graphs with local and long range links is introduced.
- Dynamical equation for reaction–diffusion processes in such graphs is presented.
- Spreading prediction is given using newly introduced topological quantities.

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ABSTRACT

We study spreading dynamics of a reaction–diffusion process in a special class of heterogeneous graphs with Poissonian degree distribution and composed of both local and long range links. The behavior of the spreading dynamics on such networks are investigated by relating them to the topological features of graphs. We find that the degree of assortativity can give just some indication about the large scale behavior of the spreading dynamics while a detailed description of the process can be addressed by introducing new, more appropriate, topological quantities linked to the distance between nodes.

1. Introduction

The study of complex networks is a recent discipline that gathers together methods from both graph theory and statistical mechanics. As a result it provides a playground for the investigation of systems coming from different disciplines ranging from physics to social science, from biology to computer science (see for example [1–4]). The interested reader can also refer to many good books describing the power of complex networks in the description of different real systems as [5–7].

Many works devoted to complex networks are descriptive (see [8] and references therein), i.e., their main interest is in the network features, such as the degree of distribution of the nodes, the scale free properties (together with its characteristic exponent), the clustering structure, the assortative or disassortative nature and so on. On the other hand, the dynamics of systems living in a network is of great interest in many contexts (see [3,4]) highlighting the importance of dynamical processes on complex networks: we can mention the works on the epidemic spreading by Pastor-Satorras et al. [9], or those on the spreading patterns of mobile phone viruses by Wang et al. [10], or the signal propagation in the protein by Chennubhotla and Bahar [11]. Moreover in chemistry, biology and social science one has to deal with active species in non-trivial substrates (see, for example, [12]). In particular, in biological systems a completely new focus have been posed on

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the complex networks, as reported by Proulx et al. [13], due to the ubiquitous appearance of network structure in living systems, i.e., gene networks, protein interaction networks, predator–prey interaction.

There are different possible approaches to the study of evolution dynamics on networks. The first family is based on a mesoscopic description of the network over which the dynamical process takes place. In some cases the network is replaced by a generalized diffusive term that takes into account the network properties as in [14]. In other cases the approach is to use mean-field dynamics that incorporate the network features as in [15]. An accurate description of evolution dynamics on networks concerns numerical simulations in which the graph structure of the network is entirely considered. Here the dynamics can be agent based, such as in the random walk model on graph (see, for example [16]), or can be population based, in which at each given time step a population living in the network evolves following a given rule, as in [17], or, finally, as in the case studied here, can be field based, in which each node of the network contains a continuous field that evolves following specific rules (diffusion and reaction terms, see [18,19]).

The paper is organized as follows: in Section 2, starting with a brief introduction of the classical reaction–diffusion problem in homogeneous systems, we immediately generalized it to the non-trivial case of heterogeneous systems, introducing reaction-transport dynamics on graphs. Section 2 is also devoted to the description of graphs involved in this work, that is heterogeneous random graphs with a Poissonian degree distribution and two different kind of links: local ones describing 1d structure, where each site is connected to its nearest neighbors, and random global ones describing long range connections between distant nodes. Section 3 introduces the observables related to the dynamics, like the percentage of filling of the system and the filling time, measuring the time needed to fill with reaction products a given percentage of the system. In this section we give a first insight on the spreading dynamic presenting a phenomenological description of the system evolution. Section 4, which studies the correlation between spreading dynamics and topological parameters of the networks, attempts to infer information about the features of the reaction spreading on graphs. One of the most relevant topological indicator often used for such a purpose is the degree of assortativity, see [20], that appears to give some hints about the spreading process, as studied in [21] in the case of scale-free networks. However, in this paper, we show that the most revealing topological characteristic of the graphs, able to predict the features of the spreading process, is a modified version of the average distance between nodes [20]. In the Conclusions final considerations and some perspectives are presented.

2. The model

2.1. Reaction–diffusion dynamics in homogeneous systems

The first model of reaction–diffusion dates back to the Fisher–Kolmogorov–Petrovskii–Piskunov (FKPP) model by Kolmogorov et al. [22,23]

$$\partial_t \theta(x) = D\Delta\theta(x) + \alpha f(\theta(x)), \tag{1}$$

where D is the molecular diffusivity, α is the reaction rate and $f(\theta)$ is a convex function ($f''(\theta) < 0$ and $f'(0) = 1$) with $f(0) = f(1) = 0$, which describes the reaction process. The scalar field θ represents the fractional concentration of the reaction products: $\theta = 0$ indicates the fresh (unstable) material, $\theta = 1$ the inert (stable) one, and $0 < \theta < 1$ means that fresh materials coexist with products. In such a system, provided that the initial concentration is zero apart from a small portion of the system where $\theta \neq 0$, at long times one observes a front connecting unstable and stable states propagating through the space, i.e., $\theta(x, t) = h(x - v_f t)$, and $h(z) \sim e^{-z/\xi}$. In this case the speed of the propagating front at long times reaches an asymptotic value, $v_0 = 2\sqrt{D\alpha}$, and the thickness of the active zone is $\xi = 8\sqrt{D/\alpha}$.

More recently, reaction-transport dynamics attracted considerable interest for their relevance in a large number of chemical, biological and physical systems (see for example [12,24,25]): the transport operator $D\Delta\theta$ has been extended in order to consider both moving media and anomalous diffusion, and the reaction term $f(\theta)$ has been generalized in order to consider various kinds of interaction between different species.

Nowadays there exist many works on the study of both complex networks and reaction-transport processes, however, despite the clear relevance of the topic, very few have been centered on the study of reactive systems in networks (see [18, 19]).

2.2. Reaction–diffusion dynamics in heterogeneous systems

Graph theory is the appropriate framework to deal with various kinds of complex and heterogeneous systems such as infrastructures, social networks and the World Wide Web, biological networks, and so on (for a comprehensive text see [7]). The common feature of these systems is the presence of nodes and connections between them, although the elements at the basis of the networks are different.

From a mathematical point of view, a graph is a set of nodes, or vertexes, $i \in V$, connected by links or edges, $(i, j) \in E$. The size of the graph is defined as the total number of nodes N_{tot}. A graph is fully defined by its adjacency matrix [26], A_{ij}, that is equal to 1, or 0, if the link (i, j) is in E, or not, respectively:

$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{if } (i,j) \notin E. \end{cases} \tag{2}$$