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Walk entropies in graphs

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ABSTRACT

Entropies based on walks in graphs and in their line graphs are defined. They are based on the summation over diagonal and off-diagonal elements of the exponential of the adjacency matrix, known as the network communicability. The walk entropies are strongly related to the walk regularity of graphs and line graphs. They are not biased by the graph size and have significantly better correlation with the inverse participation ratio of the eigenmodes of the adjacency matrix than other graph entropies. A homogeneous weighting of the edges of the graph is used to simulate the effects of the 'temperature' over the entropies defined. In particular, the walk entropy of graphs is non-monotonic for regular but non-walk-regular graphs in contrast to non-regular graphs.

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1. Introduction

With recent surge of interest in complex networks—large graphs representing the skeleton of complex systems—in various fields, many quantities have been proposed to characterize the structural properties of graphs [1,2]. Among various graph invariants, a special role has been played by the concept of entropy. Entropy measures for graphs have been used for a long time in different fields [3–7], but most of them have been introduced in *ad hoc* ways. Inspired by connections between quantum information and graph theory the von Neumann entropy for graphs has been defined [5], which in general depends on the regularity, the number of connected components, the shortest-path distance and nontrivial symmetries in the graph. This entropy is defined on the basis of the eigenvalues of the discrete Laplacian matrix L of a graph: $S = -\sum_{j=1}^{n} \mu_j \ln \mu_j$, where μ_j is an eigenvalue of L. Usually,

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the logarithm of basis 2 is used to express the entropy in bits, but we will use here natural logarithms without any loss of generality. Previously, Estrada and Hatano [6] have defined the Shannon entropy of a network by using a tight-binding Hamiltonian of the form $H = -A$, where A is the adjacency matrix of the graph. That entropy is based on the probability $p_j = \exp(\lambda_j)/Z$ of finding the graph in a state with energy given by $-\lambda_j$, where λ_j is an eigenvalue of A and $Z = \sum_{j=1}^{n} \exp(\lambda_j)$.

Here, we define graph entropies based on walks in a graph. Walks in graphs play a fundamental role in the analysis of the structure and dynamical processes in networks [8]. The new graph entropies, namely the walk entropies, account for the amount of uncertainty in selecting a walk that started (and ended) at a given node or edge of the graph. The walk entropies thereby characterize the spread of a walk among the vertices or edges of the graph; in other words, we understand by the walk entropies how much the walker is concentrated, or "localized" in just a few nodes. We show that the behavior of the walk entropies is remarkably different for walk-regular, regular and non-regular graphs. The walk entropies have their maximum for the walk-regular graphs, which include important graphs such as vertex-transitive graphs, distance-regular graphs and strongly-regular graphs [9]. Some of these graphs, namely distance-regular and strongly-regular ones, have been studied in the context of quantum information theory with different interesting properties [10–14]. We also analyze the effects of the temperature on the walk entropies and the localization in different types of graphs. We introduce the walk entropy for a graph in Section 3 and for the line graph of a graph in Section 4. In Section 5, we relate the walk entropies to the localization of a walker on the nodes and edges of a graph. Section 6 further argues the temperature effect on the relation between the walk entropies and the localization.

2. Preliminaries

Before proceeding, we summarize a few definitions which are necessary to make this paper self-contained. Let us consider here simple graphs $G = (V, E)$ with $|V| = n$ nodes and $|E| = m$ edges; no multiedges or self-loops are allowed. A walk of length k is a sequence of (not necessarily distinct) nodes $v_0, v_1, \ldots, v_{k-1}, v_k$ such that for each $i = 1, 2, \ldots, k$ there is a link from v_{i-1} to v_i. If $v_0 = v_k$, the walk is named a closed walk. The number of walks of length k from node p to node q is given by $(A^k)_{pq}$, where A is the adjacency matrix of the graph. A graph is said to be *regular* if every node has the same degree. The degree of the node p, denoted by k_p, is the number of edges incident to it. A *walk-regular graph* is a graph for which $(A^k)_{pp} = \omega(k)$ for any k and for all nodes of the graph, where ω is a certain integer number. It is known that a walk-regular graph is also regular.

In order to define graph entropies based on the walks, we consider a random walker which walks from one node to another by using the edges of the graph. This consideration is similar to the ones previously used in Ref. [10] and more recently in several works [11,12]. We identify the negative adjacency matrix as a Hamiltonian of the walker and consider the thermal Green's function of the graph as previously described by Estrada and Hatano [15]

$$G_{pp}(\beta) = \langle p|e^{-\beta H}|p\rangle = \langle p|e^{\beta A}|p\rangle, \tag{1}$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature. The temperature here is a homogeneous weight assigned to every link in the graph. It is a metaphor that measures the level of stress to which the links of the graph, particular in the case of real-world networks, are submitted. The high-temperature limit $\beta \to 0$ indicates a high level of stress in the links which decreases the communication through them to almost zero. This situation models what happen in the real world when there is a high level of social agitation in socioeconomic networks, a biological system is submitted to extreme physiological conditions or some sort of physical overexploitation is applied to engineering or infrastructural networks. The reader is referred to [1] for further explanations.

The partition function for the graph is then defined by [12,14]

$$Z(\beta) = tr\left(e^{\beta A}\right). \tag{2}$$

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