Quantifying Complexity in Networks: The von Neumann Entropy

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ABSTRACT

The authors introduce a novel entropic notion with the purpose of quantifying disorder/uncertainty in networks. This is based on the Laplacian and it is exactly the von Neumann entropy of certain quantum mechanical states. It is remarkable that the von Neumann entropy depends on spectral properties and it can be computed efficiently. The analytical results described here and the numerical computations lead us to conclude that the von Neumann entropy increases under edge addition, increases with the regularity properties of the network and with the number of its connected components. The notion opens the perspective of a wide interface between quantum information theory and the study of complex networks at the statistical level.

Keywords: Complexity, Disorder, Entropy, Networks, Regularity, Random Graphs, Scale-Free Graphs, Spectra of Graphs, Quantum Information, Quantum Mechanics

INTRODUCTION

The von Neumann entropy (or equivalently quantum entropy) was defined by von Neumann (1955) in his fundational work in quantum mechanics. Nowadays the von Neumann entropy is an important tool in quantum information theory (see Nielsen and Chuang (2001); Ohya and Petz (1993)). In the present work we first associate a graph to a quantum state injectively. Then we study the von Neumann entropy of the state itself. Since the information contained in the state is nothing more but the information contained in the graph, with an easy abuse of language, we can say that we study the von Neumann entropy of the graph.

Our purpose is to get a feeling about the properties of a network described by the Neumann entropy. During our discussion, we will guess that the properties highlighted by the entropy are related, even if not in a clear way, to the amount of symmetry in a graph. (Quantitative measures of complexity in networks have been described by Bonchev and Buck (2005).)

As a matter of fact, the notion opens the perspective of a wide interface between quantum information theory and the study of complex networks at the statistical level.

From the technical point of view, we take a straightforward approach based on a faith-
ful mapping between discrete Laplacians and quantum states, firstly introduced by Braunstein, Ghosh, and Severini (2006); see also Hildebrand, Mancini, and Severini (2008).

We interpret the set of eigenvalues of an appropriately normalized discrete Laplacian as a distribution and we compute its Shannon entropy. Let us recall that the Shannon entropy measures the amount of uncertainty of a random variable, or the amount of information obtained when its value is revealed. The topic is extensively covered by, e.g., Cover and Tomas (1991).

It is not simple to give a combinatorial interpretation to the von Neumann entropy. Superficially, we give evidence that this can be seen as a measure of regularity, i.e., regular graphs have a generally higher entropy when the number of edges has been fixed. This is not the end of the story. Quantum entropy seems to depend on the number of connected components, long paths, and nontrivial symmetries (in terms of the automorphism group of the graph).

Fixed the number of edges, entropy is smaller for graphs with large cliques and short paths, i.e., graphs in which the vertices form an highly connected cluster. The remainder of the article is organized as follows.

In the next section we introduce the required definitions and focus on first properties. By adding edges one by one to the empty graph (that is, the graph with zero edges), we attempt to construct graphs with minimum and maximum entropy, respectively.

We then explore the influence of the graph structure on the entropy. We consider different classes of graphs: regular graphs, random graphs, and the star as an extremal case of scale-free graph (i.e., graphs for which the degree distribution follows a power law). We have chosen these classes because these are well-studied and considered in many different contexts. The asymptotic behavior for large number of vertices shows that regular graphs tend to have maximum entropy.

We study numerically how the entropy increases when adding edges with different prescriptions. Once fixed the number of edges, the entropy is minimized by graphs with large cliques. In the concluding section, we will indicate a number of directions for future research.

THE VON NEUMANN ENTROPY

The state of a quantum mechanical system with a Hilbert space of finite dimension $n$ is described by a density matrix. Each density matrix $\rho$ is a positive semidefinite matrix with $\text{Tr}(\rho) = 1$. Here we consider a matrix representation based on the combinatorial Laplacian to associate graphs to specific density matrices.

Let $G = (V, E)$ be a simple undirected graph with set of vertices $V(G) = \{1, 2, \ldots, n\}$ and set of edges $E(G) \subseteq V(G) \times V(G) - \{\{v, v\} : v \in V(G)\}$. The adjacency matrix of $G$ is denoted by $A(G)$ and defined by $[A(G)]_{u,v} = 1$ if $\{u, v\} \in E(G)$ and $[A(G)]_{u,v} = 0$, otherwise.

The degree of a vertex $v \in V(G)$, denoted by $d(v)$, is the number of edges adjacent to $v$. A graph $G$ is $d$-regular if $d(v) = d$ for all $v \in V(G)$. Let $d_G \in \mathbb{N}$ be the degree-sum of the graph, i.e. $d_G = \sum_{v \in V(G)} d(v)$. The average degree of $G$ is defined by

$$d_G = n^{-1} \sum_{v \in V(G)} d(v),$$

where $n$ is the number of non-isolated vertices, that is vertices $v$ such that $\{u, v\} \in E(G)$ for some $u \in V(G)$.

The degree matrix of $G$ is an $n \times n$ matrix, denoted by $\Delta(G)$, having $uv$-th entry defined as follows: $[\Delta(G)]_{u,v} = d(v)$ if $u = v$ and $[\Delta(G)]_{u,v} = 0$, otherwise.

The combinatorial Laplacian matrix of a graph $G$ (for short, Laplacian) is the matrix $L(G) = \Delta(G) - A(G)$. The matrix $L(G)$ is a major tool for enumerating spanning trees (via the Matrix-Tree Theo. It is then clear that

$$n.$$

The entropy of a density matrix $\rho$ is defined as $S(\rho) = - \text{Tr}(\rho \log_2 \rho)$.
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