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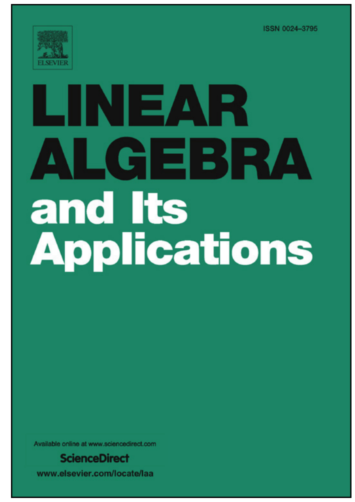

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SYMMETRIC LAPLACIANS, QUANTUM DENSITY MATRICES AND THEIR VON-NEUMANN ENTROPY

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Abstract. We show that the (normalized) symmetric Laplacian of a simple graph can be obtained from the partial trace over a pure bipartite quantum state that resides in a bipartite Hilbert space (one part corresponding to the vertices, the other corresponding to the edges). This suggests an interpretation of the symmetric Laplacian's Von Neumann entropy as a measure of bipartite entanglement present between the two parts of the state. We then study extreme values for a connected graph's generalized Rényi-p entropy. Specifically, we show that

(1) the complete graph achieves maximum entropy,
(2) the 2-regular graph:
    (a) achieves minimum Rényi-2 entropy among all k-regular graphs,
    (b) is within $\log 4/3$ of the minimum Rényi-2 entropy and $\log 4\sqrt{2}/3$ of the minimum Von Neumann entropy among all connected graphs,
    (c) achieves a Von Neumann entropy less than the star graph.

Point (2) contrasts sharply with similar work applied to (normalized) combinatorial Laplacians, where it has been shown that the star graph almost always achieves minimum Von Neumann entropy. In this work we find that the star graph achieves maximum entropy in the limit as the number of vertices grows without bound.

Keywords: Symmetric; Laplacian; Quantum; Entropy; Bounds; Rényi.

1. Introduction

In recent years, there have many attempts to increase our understanding of graph structure by studying graph entropy. Many different approaches to studying graph entropy have been proposed, and to the best of the authors' knowledge, it is not clear if/how many of these relate to each other. For example, in [1] an information function was defined in order to associate an entropic quantity with the network; in [2], the entropic properties of graph ensembles were studied; while in [3,4] Shannon entropy was used to study the topological uncertainty within spatial networks. There have also been studies of the Von Neumann (quantum) entropy [5] of graphs [2,6–17]. This work focuses on such a study.

The mathematical theory of quantum mechanics allows us to view quantum states of finite-dimensional systems as Hermitian, positive semi-definite matrices with unit trace [5]. It is also known that the combinatorial Laplacian of a graph is a symmetric positive semi-definite matrix. Thus, normalizing this matrix by its trace allows us to view the graph as a quantum state, [6]. A natural next step is to study the information content of the graph by considering the Von Neumann entropy of the graph's corresponding quantum state, [7]. In that work, it was noted that the Von Neumann entropy may be interpreted as a measure of network regularity. In [8], it was then shown that for scale free networks the Von Neumann entropy of a graph is linearly related to the Shannon entropy of the graph's ensemble. Correlations between these entropies were observed when the graph's degree distribution displayed heterogeneity in [2]. It was not until the work of [9] that a well defined operational interpretation of the graph's Von Neumann entropy was established. Specifically, in that work it was demonstrated that the Von Neumann entropy should be interpreted as the number of entangled bits that are represented by the graph's quantum state. Other studies of the Von Neuamnn entropy of combinatorial Laplacians have been performed in [10–13]. Also of interest is [14], in which it is shown that the quantum relative entropy of a graph's Laplacian with another particular quantum state can be related to the number of spanning trees of the graph.

An alternative (and seemingly less well studied) line of work has been to study the Von Neumann entropy of the *symmetric* (i.e., not combinatorial) Laplacian. In the conclusion of [7], studying the symmetric Laplacian's Von Neumann entropy was mentioned as a potential future step. In [15, 16], approximations to the symmetric Laplacian's Von Neumann entropy are established. In [17] quantum entropic measures of symmetric Laplacians are used to present an information theoretic kernel method for assessing similarities between directed graphs.