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Graph invertibility and median eigenvalues

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ABSTRACT

Let (G, w) be a weighted graph with a weight-function $w : E(G) \to \mathbb{R}\backslash\{0\}$. A weighted graph (G, w) is invertible to a new weighted graph if its adjacency matrix is invertible. Graph inverses have combinatorial interests and can be applied to bound median eigenvalues of graphs such as have physical meanings. In this paper, we characterize the inverse of a weighted graph based on its Sachs subgraphs that are spanning subgraphs with only K_2 or cycles (or loops) as components. The characterization can be used to find the inverse of a weighted graph based on its structures instead of its adjacency matrix. If a graph has its spectra split about the origin, i.e., half of eigenvalues are positive and half of them are negative, then its median eigenvalues can be bounded by estimating the largest and smallest eigenvalues of its inverse. We characterize graphs with a unique Sachs subgraph and prove that these graphs has their spectra split about the origin if they have a perfect matching. As applications, we show that the median eigenvalues of stellated graphs of trees

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and corona graphs belong to different halves of the interval $[-1, 1]$.

1. Introduction

In this paper, graphs may contain loops but no multiple edges. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Its adjacency matrix $\mathbb{A}$ is defined as the ij-entry $(\mathbb{A})_{ij} = 1$ if $ij \in E(G)$ and $(\mathbb{A})_{ij} = 0$ otherwise. Assume that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ where $n = |V(G)|$, are the eigenvalues of $\mathbb{A}$ (also the eigenvalues of G). In Quantum Chemistry, the eigenvalues of a molecular graph have physical meanings. For example, the sum of absolute value of eigenvalues of a graph G, also called the *energy* of G [13], is often equal to the total Hückel π-electron energy of the molecule represented by G. Also many physico-chemical parameters of molecules are determined by or are dependent upon the HOMO-LUMO gap [4,6], which is often given as the difference between the median eigenvalues, $\lambda_H - \lambda_L$, where $H = \lfloor (n+1)/2 \rfloor$ and $L = \lceil (n+1)/2 \rceil$.

Throughout the more traditional chemical literature, there has been extensive effort to deal with the HOMO-LUMO gap mostly in an explicit consideration of individual molecules case by case. A few mathematical methods have been developed especially in the last decade to characterize the HOMO-LUMO gaps of graphs in a general manner [5,9,11,12,17–19,27]. Recently, Mohar introduced a graph partition method to bound the HOMO-LUMO gaps for subcubic graphs [17–19]. However, not all graphs have these nice partition properties and a desired partition is hard to find, even for plane subcubic graphs [17].

It is well-known that the eigenvalues of a bipartite graph are symmetric about the origin. If the adjacency matrix $\mathbb{A}$ of a bipartite graph G is invertible, then the reciprocal of the maximum eigenvalue of $\mathbb{A}^{-1}$ is equal to the λ_H of G and the reciprocal of the least eigenvalue of $\mathbb{A}^{-1}$ is equal to λ_L. Based on this fact, the invertibility of adjacency matrices of trees had been discussed in order to evaluate their HOMO-LUMO gaps [5,9], and later the method has been extended to bipartite graphs with a unique perfect matching [11,21]. Besides the chemical interests, the invertibility of adjacency matrices of graphs is of independent interest as indicated in [5,16]. For examples, the invertibility of adjacency matrices of graphs has connections to other interesting combinatorial topics such as Möbius inversion of partially ordered sets (see the treatment in Chapter 2 of Lovász [14]) [5,21] and Motzkin numbers [2,16].

Here, the aim of this paper is to extend this idea to graphs with more general settings. Note that, the eigenvalues of non-bipartite graphs are not symmetric about the origin. But, the above methodology works when the eigenvalues of a graph evenly split about the origin, i.e., half of them are positive and half of them are negative. Another purpose of this paper is to discuss the invertibility of graphs. The inverse of the adjacency matrix of