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On a construction of integrally invertible graphs and their spectral properties

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A B S T R A C T

Godsil (1985) defined a graph to be invertible if it has a non-singular adjacency matrix whose inverse is diagonally similar to a nonnegative integral matrix; the graph defined by the last matrix is then the inverse of the original graph. In this paper we call such graphs positively invertible and introduce a new concept of a negatively invertible graph by replacing the adjective 'nonnegative' by 'nonpositive in Godsil's definition; the graph defined by the negative of the resulting matrix is then the negative inverse of the original graph. We propose new constructions of integrally invertible graphs (those with non-singular adjacency matrix whose inverse is integral) based on an operation of 'bridging' a pair of integrally invertible graphs over subsets of their vertices, with sufficient conditions for their positive and negative invertibility. We also analyze spectral properties of graphs arising from bridging and derive lower bounds for their least positive eigenvalue. As an illustration we present a census of graphs with a unique 1-factor on $m \leq 6$ vertices and determine their positive and negative invertibility.

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1. Introduction

A number of ways of introducing inverses of graphs have been proposed, all based on inverting adjacency matrices. For a graph with a non-singular adjacency matrix a first thought might be to hope that the inverse matrix defines a graph again. It turns out, however, that this happens to be the case only for unions of isolated edges [6]. A successful approach was initiated by Godsil [4] who defined a graph to be invertible if the inverse of its (non-singular) adjacency matrix is diagonally similar (cf. [15]) to a nonnegative integral matrix representing the adjacency matrix of the inverse graph in which positive labels determine edge multiplicities. This way of introducing invertibility has the appealing property that inverting an inverse graph gives back the original graph. For a survey of results and other approaches to graph inverses we recommend [9].

Inverse graphs are of interest in estimating the least positive eigenvalue in families of graphs, a task for which there appears to be lack of suitable bounds. However, if the graphs are invertible, one can apply one of the (many) known upper bounds on largest eigenvalues of the inverse graphs instead (cf. [10–12]). Properties of spectra of inverse graphs can also be used to estimate the difference between the minimal positive and maximal negative eigenvalue (the so-called HOMO-LUMO gap) for structural models of chemical molecules, as it was done e.g. for graphene in [14].

Godsil's ideas have been further developed in several ways. Akbari and Kirkland [7] and Bapat and Ghorbani [1] studied inverses of edge-labeled graphs with labels in a ring, Ye et al. [13] considered connections of graph inverses with median eigenvalues, and Pavlíková [10,12] developed constructive methods for generating invertible graphs by edge overlapping. A large number of related results, including a unifying approach to inverting graphs, were proposed in a recent survey paper by McLeman and McNicholas [9], with emphasis on inverses of bipartite graphs and diagonal similarity to nonnegative matrices.

Less attention has been given to the study of invertibility of non-bipartite graphs and their spectral properties which is the goal of this paper. After introducing basic concepts, in Section 2 we present an example of a non-bipartite graph representing an important chemical molecule of fulvene. Its adjacency matrix has the remarkable additional property that its inverse is integral and diagonally similar to a nonpositive rather than a nonnegative matrix. This motivated us to introduce negative invertibility as a natural counterpart of Godsil [4] concept: A negatively invertible graph is one with a non-singular adjacency matrix whose inverse is diagonally similar to a nonpositive matrix. The negative of this matrix is then the adjacency matrix of the inverse graph. Positively and negatively invertible graphs are subfamilies of integrally invertible graphs, whose adjacency matrices have an integral inverse. The corresponding inverse graphs, however, would have to be interpreted as labeled graphs with both positive and negative (integral) edge labels.

Results of the paper are organized as follows. In Section 3 we develop constructions of new integrally invertible graphs from old ones by 'bridging' two such graphs over