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INVERSES OF TREES

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Let T be a tree with a perfect matching. It is known that in this case the adjacency matrix A of T is invertible and that A^{-1} is a (0, 1, -1)-matrix. We show that in fact A^{-1} is diagonally similar to a (0, 1)-matrix, hence to the adjacency matrix of a graph. We use this to provide sharp bounds on the least positive eigenvalue of A and some general information concerning the behaviour of this eigenvalue. Some open problems raised by this work and connections with Möbius inversion on partially ordered sets are also discussed.

1. Introduction

This paper was motivated by a question in Chemistry; nevertheless the graph theory resulting seems to be of independent interest.

Suppose G is a bipartite graph with adjacency matrix A. In a simple model in Quantum Chemistry, the eigenvalues of A have a physical meaning and so the relation between the graph theoretic properties of G and the eigenvalues of A are of some interest. If G is bipartite then the eigenvalues of A are symmetrically placed about the origin. In the cases of most chemical importance A must be non-singular, hence A must have even order. Suppose G has $2m$ vertices. Thus A will have exactly m positive eigenvalues and m negative eigenvalues.

One of the most important of these eigenvalues turns out to be the mth one — i.e. the least positive eigenvalue. Theoretically its magnitude is expected to be correlated with the amount of energy needed to remove an electron from the hydrocarbon molecule represented by G (for further information see e.g. [9]). Information about the magnitude of this eigenvalue is not easily gained in general. Ivan Gutman has suggested the following conjecture: amongst all trees on $2m$ vertices having perfect matchings, the path has smallest least positive eigenvalue. (The adjacency matrix of a tree is invertible iff the tree has a perfect matching.)

In this paper we show that Gutman's conjecture is correct and obtain sharp bounds on the magnitude of the eigenvalue in question. Furthermore, noting that a tree with a perfect matching has just one perfect matching leads us to consider, and solve, the corresponding problem for a slightly more general class of graphs.

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We are lead incidentally to some interesting graph theory. We show that if T is a tree with invertible adjacency matrix A then there is a diagonal matrix Φ such that $\Phi^{-1}A^{-1}\Phi$ is non-negative (0, 1)-matrix. Thus the inverse of A is essentially the adjacency matrix of a graph. (The diagonal entries of Φ are each $+1$ or -1.)

The fact that, when T is a tree, $A(T)^{-1}$ is a $(0, 1, -1)$-matrix has been noted previously. It is stated explicitly as Lemma 1 in [4] and is implicit in [5: Equation (42)] and [8: Theorem 1]. Our contribution is the observation that A^{-1} is essentially a non-negative matrix and that this has non-trivial consequences concerning the behaviour of the least positive eigenvalue.

Finally it should be noted that there is a connection between the inversion problem considered and Möbius inversion on partially ordered sets. This is discussed at some length in the final section of this paper, along with some open questions raised by our results.

2. Inverses

Let G be a bipartite graph. We say (R, C) is a *bipartition* of G if the sets R and C partition $V(G)$ into independent sets. Given a bipartition of G we define the *incidence matrix* $B=B(G)$ by defining B_{ij} to be 1 or 0 according as the i-th vertex in R and the j-th vertex in C are adjacent or not. Clearly B depends on the bipartition of G chosen and, given this, on the ordering of the vertices within the components of the bipartition. This ambiguity will cause no problems.

Given $B=B(G)$ we can write the adjacency matrix $A=A(G)$ or partitioned form as

$$\begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}.$$

It follows in particular that A is invertible iff B is.

If B_1 and B_2 are matrices of the same order we say B_2 *dominates* B_1 if B_2-B_1 is non-negative.

Lemma 2.1. *Let G be a bipartite graph with bipartition (R, C). Then G has a unique perfect matching iff the vertices in R and C can be ordered so that $B=B(G)$ is a lower triangular matrix, with all its diagonal entries equal to one.*

Proof. We begin with the sufficiency. It is easily checked that in this case G has a perfect matching and that if G has a second perfect matching then $B(G)$ would not be lower triangular. (Any perfect matching of G determines a permutation matrix dominated by B.)

Assume now that G has a unique perfect matching M. Set $R=\{1, ..., m\}$. If $i\in R$ let i' be the unique element of C such that $\{i, i'\}\in M$. From Theorem II.1.1 of [2] (for example) we know that there is vertex in R with valency one. Denote this vertex by 1. Then deleting 1 and $1'$ from G leaves us with a bipartite graph G' with a unique perfect matching. By induction we may assume $B(G')$ is lower triangular with non-zero diagonal entries and it follows imediately that $B(G)$ also has this form. ∎

It is easy to see using Lemma 2.1 that if G is a bipartite graph with a unique perfect matching then $B(G)$ (and hence $A(G)$) is invertible. We will use this observation without explicit mention from now on.

Some further terminology is needed. Suppose G is a graph with a unique perfect matching M. We define G/M to be the graph obtained by contracting each edge of M to a single vertex. (Thus G/M is a contraction of G in in the usual sense of the term.)

Theorem 2.2. *Let G be a bipartite graph with a unique perfect matching M. Let $B=B(G)$. If G/M is bipartite then B^{-1} is diagonally similar to a non-negative integral matrix B^+ which dominates B. Furthermore if G is a forest then B^+ is* (0, 1)*-matrix.*

Proof. Let $m=|M|$ and assume $m\geqq 2$. Then we may write B in the form

$$\begin{bmatrix} C & 0 \\ b^T & 1 \end{bmatrix}$$

where C is an $(m-1)\times(m-1)$ lower triangular matrix with all diagonal entries equal to one. Let (R_0, R_1) be a bipartition of G/M. Assume $R=\{v_1, \ldots, v_m\}$ and that $v_m\in R_0$. Let Φ be the $m\times m$ diagonal matrix with i-th diagonal entry equal 1 if $v_i\in R_0$ and equal -1 otherwise. Let Φ_m be the matrix obtained by deleting the last row and column from Φ.

Then $\Phi B^{-1}\Phi$ can be written as

$$\begin{bmatrix} \Phi_m C^{-1}\Phi_m & 0 \\ -b^T C^{-1}\Phi_m & 1 \end{bmatrix}.$$

Applying our theorem inductively we may assume that $\Phi_m C^{-1}\Phi_m$ is non-negative. We have $b^T C^{-1}\Phi_m = b^T\Phi_m \Phi_m C^{-1}\Phi_m$. Since $v_m\in R_0$ and G/M is bipartite, each vertex v_i adjacent to v_m in G/M is in R_1. From our definition of Φ it follows that $-b^T\Phi_m$ is non-negative. Accordingly $\Phi B^{-1}\Phi$ is non-negative.

Since $\Phi^{-1}=\Phi$ we thus have $B^+=\Phi B^{-1}\Phi$. By induction we may assume $\Phi_m C^{-1}\Phi_m$ dominates C. As the diagonal entries of $C^{-1}\Phi_m$ are all non-zero it follows that $-b^T C^{-1}\Phi_m$ dominates b. Thus B^+ dominates B as claimed. It only remains for us to check that B^+ is $0-1$ if G is a forest.

This can be proved inductively, along with the non-negativity of $\Phi B^{-1}\Phi$. (Take v_m above to be an end-vertex, in which case b has exactly one non-zero entry and so $-b^T C^{-1}\Phi_m$ is a (0, 1)-vector). However we leave the details as an exercise since in [4], Cvetković et al prove that the inverse of the adjacency matrix of a forest (if it exists) is a (0, 1, -1)-matrix. The adjacency matrix of a forest is invertible iff the forest has a perfect matching (see e.g. [3: Theorem 1.3] or [11: Exercise 11.4]). As any graph with two perfect matching contains a cycle, a forest has at most one perfect matching. ∎

The fact that, for forests, B^+ dominates B was first noted in [4: Lemma 3]. Also both equation (42) in [5] and Theorem 1 in [10] imply that $A(G)^{-1}$ is a (0, 1, -1)-matrix when G is acyclic.

The matrix B^+ in the previous theorem may be viewed as the incidence matrix of a bipartite multigraph G^+. We will call G^+ the *inverse* of G. (We will only refer to inverses when G is bipartite with a unique perfect matching M and G/M is bipartite.) Since B^+ dominates B we can view G as a spanning subgraph of G^+. However, something even more surprising is true.

Suppose first that G is a forest with a unique perfect matching and that G has $2m$ vertices. Let P_{2m} denote the path with $2m$ vertices. Then G^+ is a spanning subgraph of P_{2m}^+. This holds because (a) if $B=B(G)$ then B^+ is a (0, 1)-matrix, and (b) if $F_{2m}=B(P_{2m})$ then F_{2m}^+ is a lower triangular matrix with each entry on or below the diagonal equal to one. Here we assume the vertices of P_{2m} are labelled $1, m+1, 2, m+2, \ldots$. The proof of our claim is easily established by induction and will be left as an exercise.

More can be said. Let $E=E_{2m}$ be the bipartite graph with $B=B(E)$ given by:

$$(B)_{ij}=\begin{cases}0 & i<j \quad \text{or} \quad i-j \quad \text{is even}\\ 1 & \text{otherwise.}\end{cases}$$

Lemma 2.3. *Let G be a connected bipartite graph on $2m$ vertices. Assume G has a unique perfect matching M and that G/M is bipartite. Let $B=B(G)$. Then B^+ is dominated by $B(E)^+$.*

Proof. We leave the reader the interesting task of showing that E_m^+ has ij-entry equal to $f(i+j-3)$, where $f(k)$ is the k-th Fibonacci number, (so $f(2)=2$). Assume G satisfies out hypotheses and write B as

$$\begin{bmatrix} C & 0\\ b^T & 1\end{bmatrix}.$$

Thus B^{-1} equals

$$\begin{bmatrix} C^{-1} & 0\\ -b^TC^{-1} & 1\end{bmatrix}.$$

Let (R_0, R_1) be the bipartition of G/M.

By induction we may assume that, unless $i=1$ and $j=m$, $(B^+)_{ij}\leqq f(i+j-3)$. (Note that we can apply induction to the matrix resulting when the last row and column of B are deleted, as well as to C.) Let $\beta=(B^+)_{mi}$, and let $-\Sigma_0(C)$ and $\Sigma_1(C)$ be the sum of the positive and negative entries respectively of the first column of C^{-1}. Since all entries of this column corresponding to vertices in R_0 are non-negative and the remaining entries are non-positive, it follows that $\beta\leqq\max\{\Sigma_0(C), \Sigma_1(C)\}$. We will now prove inductively that

$$\max\{\Sigma_0(B), \Sigma_1(B)\}\leqq f(m-2)$$

$$\min\{\Sigma_0(B), \Sigma_1(B)\}\leqq f(m-3),$$

assuming that these statements hold with C and $m-1$ in place of B and m respectively.

Let v be the vertex of G corresponding to the last row of B. If $v\in R_0$ then $\beta\leqq\Sigma_1(C)$ and so

$$\Sigma_0(B)\leqq\Sigma_0(C)+\Sigma_1(C).\ \Sigma_1(b)=\Sigma_1(C).$$

If $v\in R_1$ we have instead

$$\Sigma_0(B)=\Sigma_0(C).\ \Sigma_1(B)\leqq\Sigma_0(C)+\Sigma_1(C).$$

Since $f(m-3)+f(m-4)=f(m-2)$ this proves our claims. ∎

3. Applications

We will now apply the results of the previous section to obtain bounds on the least positive eigenvalue of graphs in the classes considered there. We need some new notation first. The i-th largest eigenvalue of (the adjacency matrix of) a graph will be denoted by $\lambda_i(G)$. If G is bipartite with $2m$ vertices and $B=B(G)$ then we see that B is invertible iff $\lambda_m(G)>0$ (because the eigenvalues of a bipartite graph are symmetrically placed about the origin). We recall that if H is a subgraph of graph G then $\lambda_1(H)\leqq\lambda_1(G)$ and that if H is proper and G is connected then $\lambda_1(H)<\lambda_1(G)$. (For these results see e.g [3: Theorem 0.6].)

Theorem 3.1. *Let G be a connected bipartite graph with a unique perfect matching M such that G/M is bipartite. Assume G has $2m$ vertices. Then:*

(a) $\lambda_1(G)\lambda_m(G) \leqq 1$, *with equality iff* $G = G^+$.

(b) $\lambda_m(G) \geqq \lambda_m(E_{2m})$, *with equality iff* $G \cong E_{2m}$.

(c) *If G is a forest* $\lambda_m(G) \leqq \lambda(P_{2m})$, *with equality iff* $G \cong P_{2m}$.

Proof. By Theorem 3.2, B^+ is similar to B^{-1}. Hence $\lambda_1(G^+)=1/\lambda_m(G)$. Since B^+ dominates B we have $\lambda_1(G)\leqq\lambda_1(G^+)$, which proves (a). From Lemma 2.3 we see that $B(E_{2m})^+$ dominates B^+, proving that $1/\lambda_m(G)\leqq 1/\lambda_m(E_{2m})$ and thus yielding (b). Finally by our remarks following the proof of 3.2 we know that if G is a forest then $B(P_{2m})^+$ dominates B^+ and so (c) follows. ∎

I have not been able to characterize the graphs with $G\cong G^+$. However if G is a tree then it follows from [6: Theorem 3.2] that $G=G^+$ iff G can be constructed from a tree T on m vertices by joining a new end-vertex to each vertex in T. (So $T=P_2$ gives $G=P_4$).

A good approximation to $\lambda_m(E_{2m})$ follows on observing that $\lambda_1(E_{2m}^+)$ is bounded below by the average row sum of $B(E_{2m})^+$ and bounded above by the maximum row sum. This yields

$$1/f_{m-1} \leqq \lambda_m(E_{2m}) \leqq m/f_m,$$

whence we deduce that $[\lambda_m(E_{2m})]^{1/m}$ tends to $(\sqrt{5}-1)/2$ as m increases. It is well known (see e.g. [11: Exercise 11.5]) that $\lambda_m(P_{2m})=2\cos\left(m\pi/(2m+1)\right)$ which is asymptotically of order $\pi/2m$. The big difference in behaviour of $\lambda_m(E_{2m})$ and $\lambda_m(P_{2m})$ is a little unexpected. It is also surprising that, if G is a tree on $2m$ vertices with a perfect matching then $\lambda_m(G)\geqq\lambda_m(P_{2m})$, $\lambda_1(G)\geqq\lambda_1(P_{2m})$ (see [12]) but

$$\sum_{i=1}^{m}\lambda_i(G) \leqq \sum_{i=1}^{m}\lambda_i(P_{2m})$$

(see [8]).

Some information about the eigenvector of $A(G)$ associated with $\lambda_m(G)$ can also be obtained. The key points are (i) A and A^{-1} have the same eigenvectors (ii) $1/\lambda_m(G)$ is the spectral radius of A^{-1}. Since we know there is a diagonal matrix Λ with diagonal entries ± 1 such that $\Lambda A^{-1}\Lambda$ is non-negative, the Perron—Frobenius theorems apply. If z is an eigenvector of A associated with λ_m then Λz is an eigenvector of A^+ associated with $1/\lambda_m$. But Az is the Perron vector and so if G is connected we have:

(a) λ_m is a simple eigenvalue of G. (Note that G^+ is connected if G is, since G is isomorphic to a spanning subgraph of G^+.)

(b) if H is a subgraph of G and $H \cap M$ is a perfect matching in H then $\lambda_m(H) \geqq \lambda_m(G)$.

(c) all entries of z are non-zero (and the sign of an entry is determined by the colour class of G/M in which it lies). These claims are all easily proved, but we will leave the details as an exercise.

If B is an $n \times n$ triangular (0, 1)-matrix then a simple induction argument along the lines of the proof of Lemma 2.3 shows that the maximum absolute value of an entry of B^{-1} is less than 2^{n-1}. From this it follows that if G is bipartite on $2m$ vertices and has a unique perfect matching then $\lambda_m^{1/m}(G) \geqq 1/2$.

4. An open problem

Our results lead to the following.

Problem 4.1. Characterize the bipartite graphs G with unique perfect matchings such that $B(G)^{-1}$ is diagonally similar to a non-negative matrix.

Let us call a graph G "good" if it is bipartite with a unique perfect matching and $B(G)^{-1}$ has the properties stated above. Suppose now G is a tree with a unique perfect matching. Then it is easily checked that G^+ is good. In particular P_{2m}^+ is good and P_{2m}^+/M is the complete graph on m vertices — as far as possible from being bipartite! Another interesting class of graphs can be constructed using the Kronecker product of matrices.

Suppose G_1 and G_2 are good graphs. There is a well-defined graph H with $B(H) = B(G_1) \otimes B(G_2)$. (Note: if $B = (b_{ij})$ then $B \otimes C$ is got by replacing each entry b_{ij} with the matrix $b_{ij}C$). Since $(B \otimes C)^{-1} = B^{-1} \otimes C^{-1}$, it is easy to prove that if G_1 and G_2 are good, so is H. In particular $B(P_{2m}) \otimes B(P_{2m})$ $(m \geqq 2)$ gives a good graph with non-bipartite contraction. We point out here that $B(G_1) \otimes B(G_2)$ and $B(G_1) \otimes B(G_2)^T$ are isomorphic only if G_1 or G_2 admits an automorphism swapping the colour classes.

If G is good and M is its unique perfect matching then any subgraph H of G such that $H \cap M$ is a perfect matching can be shown to be good. Thus we now have three techniques for constructing new good graphs from old ones. This seems to indicate that our Problem 4.1 will not have a simple solution.

Finally we must point out that the problems we have been considering are related to Möbius inversion. (For any unexplained terminology here see e.g. Aigner's book [1].) Let $P = \{x_1, \ldots, x_m\}$ be a poset and let $Z = Z(P)$ be the matrix with

$$Z_{ij} = \begin{cases} 1 & x_i \leqq x_j \\ 0 & x_i \not\leqq x_j. \end{cases}$$

Then (Z_{ij}^{-1}) is the value of the Möbius function on the interval $[x_i, x_j]$ in P, when this interval is non-empty (i.e. $x_i \leqq x_j$), and is zero otherwise. (The standard descriptions of Möbius inversion tend to avoid explicit mention of matrices, however the treatment in Chapter 2 of Lovász [11] makes our point clear.) If P is a geometric lattice or the face-lattice of a convex polytope then Z^{-1} is diagonally similar to a non-negative matrix Z^+ and Z^+ dominates Z (see 4.34 Corollary (iv) in [1] for geometric lattices and [7] for polytopes).

More generally it is enough to require that any interval of P is a semimodular lattice, since the Möbius function is zero on any interval which is not complemented and a complemented semimodular lattice is geometric. It is an interesting and easy exercise to show that if T is a tree with a perfect matching then $B(T^+)$ is in fact the incidence matrix of a poset where all intervals are chains, and so is distributive (and a fortiori semimodular). Hence in this case Theorem 2.2 follows from Möbius inversion.

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