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On the largest eigenvalue of the distance matrix of a bipartite graph

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Abstract

We obtain the lower and upper bounds on the largest eigenvalue of the distance matrix of a connected bipartite graph and characterize those graphs for which these bounds are best possible.

1 Introduction

Since the distance matrix and related matrices, based on graph-theoretical distances [1], are rich sources of many graph invariants (topological indices) that have found use in structure-property-activity modeling [2, 3, 4], it is of interest to study spectra and polynomials of these matrices [5, 6].

Let $G = (V, E)$ be a simple connected bipartite graph with vertex set $V(G) = \{1, 2, \ldots, n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. For $i \in V$, d_i is the degree of the i-th vertex of G, $i = 1, 2, \ldots, n$. The minimum vertex degree is denoted by δ. The diameter of a graph is the maximum distance between any two vertices of G. Let d be the diameter of G. The distance matrix $D(G)$ of G is an $n \times n$ matrix $(d_{i,j})$ such that $d_{i,j}$ is just the distance (i.e., the number of edges of a shortest path) between the vertices i and j in G [1].

Since $D(G)$ is a real symmetric matrix, its all eigenvalues are real. Let $\lambda(G)$ be the largest eigenvalue of $D(G)$. Balaban et al. [7] proposed the use of $\lambda(G)$ as a structure-descriptor, and it was successfully used to make inferences about the extent of branching and boiling points of alkanes [7, 8]. Balasubramanian [9] computed the spectrum of its distance matrix using the Givens-Householder method. In [10], the distance polynomials (that is, the characteristic polynomials of the distance matrices) were computed for several graphs. There exists a vast literature that studies the spectral radius of the distance matrix. We refer the reader to [11, 12, 13, 14] for surveys and more informations.

In this note we report the lower and upper bounds on the largest eigenvalue of the distance matrix of a connected bipartite graph and characterize those graphs for which these bounds are best possible.

2 Spectral radius of distance matrix of bipartite graph

It is a result of Perron-Frobenius in matrix theory (see [15], Page no. 66) which states that a non-negative matrix B always has a non-negative characteristic value r such that the modulii of all the characteristic values of B do not exceed r. To this 'maximal' characteristic value r there corresponds a non-negative characteristic vector

$$B\mathbf{Y} = r\mathbf{Y} \quad (\mathbf{Y} \geq 0,\ \mathbf{Y} \neq 0)\ .$$

If G is a connected graph then all the eigencomponents corresponding to the largest eigenvalue of $D(G)$ are positive.

Now we give a lower bound on the spectral radius of distance matrix of a bipartite graph.

Theorem 2.1. *Let $G = (V, E)$ be a connected bipartite graph of order n with bipartition $V(G) = A \cup B$, $|A| = p$, $|B| = q$. Then*

$$\lambda(G) \geq n - 2 + \sqrt{n^2 - 3pq}\,, \tag{1}$$

with equality holds if and only if G is a complete bipartite graph $K_{p,q}$.

Proof: Since $V(G) = A \cup B$ and $A \cap B = \Phi$, $|A| = p$, $|B| = q$, we can assume that $A = \{1, 2, \ldots, p\}$ and $B = \{p+1, p+2, \ldots, p+q\}$, where $p+q = n$. Let $\mathbf{X} = (x_1, x_2, \ldots, x_n)^T$

be an eigenvector of $D(G)$ corresponding to the largest eigenvalue $\lambda(G)$. Then we have $D(G)\mathbf{X} = \lambda(G)\mathbf{X}$. We can assume that $x_i = \min_{k\in A} x_k$, and $x_j = \min_{k\in B} x_k$. For $i \in A$,

$$\begin{aligned} \lambda(G)x_i &= \sum_{k=1,k\neq i}^{p} d_{i,k}x_k + \sum_{k=p+1}^{p+q} d_{i,k}x_k \\ &\geq 2(p-1)x_i + qx_j \ . \end{aligned} \tag{2}$$

For $j \in B$,

$$\begin{aligned} \lambda(G)x_j &= \sum_{k=1}^{p} d_{j,k}x_k + \sum_{k=p+1,k\neq j}^{p+q} d_{j,k}x_k \\ &\geq px_i + 2(q-1)x_j \ . \end{aligned} \tag{3}$$

Since G is a connected graph, $x_k > 0$ for all $k \in V$. From (2) and (3), we get

$$(\lambda(G) - 2(p-1))(\lambda(G) - 2(q-1)) \geq pq \quad \text{as } x_i,\ x_j > 0\,,$$

that is,

$$\lambda^2(G) - 2(p+q-2)\lambda(G) + 3pq - 4p - 4q + 4 \geq 0\ .$$

From this we get the required result (1).

Now suppose that equality holds in (1). Then all inequalities in the above argument must be equalities. From equality in (2), we get

$$x_k = x_j \text{ and } ik \in E(G), \quad \text{for all } k \in B\ .$$

From equality in (3), we get

$$x_k = x_i \text{ and } jk \in E(G), \quad \text{for all } k \in A\ .$$

Thus each vertex in each set is adjacent to all the vertices on the other set and vice versa. Hence G is a complete bipartite graph $K_{p,q}$.

Conversely, one can easily to see that (1) holds for complete bipartite graph $K_{p,q}$. □

Now we give an upper bound on the spectral radius of distance matrix of a bipartite graph.

Theorem 2.2. *Let $G=(V,E)$ be a connected bipartite graph of order n, diameter d with bipartition $V(G)=A\cup B$, $|A|=p$, $|B|=q$. Then*

$$\lambda(G)\leq\frac{1}{2}\left(d(n-2)+\sqrt{d^2n^2-4pq(2d-1)}\right)\tag{4}$$

for d even, and

$$\lambda(G)\leq\frac{1}{2}\left((d-1)(n-2)+\sqrt{(d-1)^2n^2-4(d-1)^2(pq-\delta^2)+4d^2pq-4d(d-1)\delta n}\right)\tag{5}$$

for d odd. Moreover, the equality holds in (4) if and only if G is a complete bipartite graph $K_{p,q}$.

Proof: Since $V(G)=A\cup B$ and $A\cap B=\Phi$, $|A|=p$, $|B|=q$, we can assume that $A=\{1,2,\ldots,p\}$ and $B=\{p+1,p+2,\ldots,p+q\}$, where $p+q=n$. Let $\mathbf{X}=(x_1,x_2,\ldots,x_n)^T$ be an eigenvector of $D(G)$ corresponding to the largest eigenvalue $\lambda(G)$. Then we have $D(G)\mathbf{X}=\lambda(G)\mathbf{X}$. We can assume that $x_i=\max_{k\in A}x_k$, and $x_j=\max_{k\in B}x_k$. For $i\in A$,

$$\lambda(G)x_i=\sum_{k=1,k\neq i}^{p}d_{i,k}x_k+\sum_{k=p+1}^{p+q}d_{i,k}x_k\ .\tag{6}$$

From (6), we get

$$\lambda(G)x_i\leq d(p-1)x_i+(d-1)qx_j\ \text{ for } d \text{ even},\tag{7}$$

$$\text{and}\qquad\lambda(G)x_i\leq(d-1)(p-1)x_i+d_ix_j+d(q-d_i)x_j\ \text{ for } d \text{ odd},\tag{8}$$

where d_i is the degree of the vertex i. For $j\in B$,

$$\lambda(G)x_j=\sum_{k=1}^{p}d_{j,k}x_k+\sum_{k=p+1,k\neq j}^{p+q}d_{j,k}x_k\ .\tag{9}$$

From (9), we get

$$\lambda(G)x_j\leq(d-1)px_i+d(q-1)x_j\ \text{ for } d \text{ even},\tag{10}$$

$$\text{and}\qquad\lambda(G)x_j\leq d_jx_i+d(p-d_j)x_i+(d-1)(q-1)x_j\ \text{ for } d \text{ odd},\tag{11}$$

where d_j is the degree of the vertex j. Since G is a connected graph, $x_k>0$ for all $k\in V$. From (7) and (10), we get

$$(\lambda(G)-d(p-1))(\lambda(G)-d(q-1))\leq pq(d-1)^2\ \text{ as } x_i,\ x_j>0\,,$$

that is,

$$\lambda^2(G) - d(p+q-2)\lambda(G) + d^2 - pq - (p+q)d^2 + 2dpq \leq 0 \quad \text{for } d \text{ even.} \tag{12}$$

Similarly, from (8) and (11), we get

$$\begin{aligned} \Big(\lambda(G) - (d-1)(p-1)\Big)\Big(\lambda(G) - (d-1)(q-1)\Big) &\leq \Big(dq - (d-1)d_i\Big)\Big(dp - (d-1)d_j\Big) \\ &\leq \Big(dq - (d-1)\delta\Big)\Big(dp - (d-1)\delta\Big), \end{aligned}$$

as $d_i, d_j \geq \delta$, that is,

$$\lambda^2(G) - (d-1)(n-2)\lambda(G) + (d-1)^2(pq + 1 - n - \delta^2) - d^2pq + d(d-1)\delta n \leq 0 \quad \text{for } d \text{ odd.} \tag{13}$$

From (12) and (13), we get the required result (4) and (5), respectively.

Now suppose that equality holds in (4). Then the equality holds in (7) and (10). From equality in (7), we get

$$d = 2,\ x_k = x_j \text{ and } ik \in E(G), \quad \text{for all } k \in B\,,$$

and

$$x_k = x_i, \quad \text{for all } k \in A\ .$$

From equality in (10), we get

$$d = 2,\ x_k = x_i \text{ and } jk \in E(G), \quad \text{for all } k \in A\,,$$

and

$$x_k = x_j, \quad \text{for all } k \in B\ .$$

Thus each vertex in each set is adjacent to all the vertices on the other set and vice versa. Hence G is a complete bipartite graph $K_{p,q}$.

Conversely, one can easily see that (4) holds for complete bipartite graph $K_{p,q}$. $\square$

Remark 2.3. *The lower and upper bounds given by (1) and (4), respectively, are equal when G is a complete bipartite graph $K_{p,q}$ and diameter d is even.*

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References

[1] D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, Graph Theoretical Matrices in Chemistry, Mathematical Chemistry Monographs No. 3; University of Kragujevac: Kragujevac, 2007.

[2] Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, N. Trinajstić, The distance matrix in chemistry, J. Math. Chem. **11** (1992) 223–258.

[3] J. Devillers, A. T. Balaban, Eds. Topological indices and related Descriptors in QSAR and QSPR; Gordon and Breach: Amsterdam, 1999.

[4] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors; Wiley-VCH: Weinheim, 2000.

[5] W. Yan, Y.-N. Yeh, F. Zhang, On the matching polynomials of graphs with small number of cycles of even length, Int. J. Quantum. Chem. **105** (2005) 124–130.

[6] X. Guo, D. J. Klein, W. Yan, Y.-N. Yeh, Hyper-Wiener vector, Wiener matrix sequence, and Wiener polynomial sequence of a graph, Int. J. Quantum. Chem. **106** (2006) 1756–1761.

[7] A. T. Balaban, D. Ciubotariu, M. Medeleanu, Topological indices and real number vertex invariants based on graph eigenvalues or eigenvectors, J. Chem. Inf. Comput. Sci. **31** (1991) 517–523.

[8] I. Gutman, M. Medeleanu, On the structure-dependence of the largest eigenvalue of the distance matrix of an alkane, Indian J. Chem. A **37** (1998) 569–573.

[9] K. Balasubramanian, A topological analysis of the C60 buckminsterfullerene and C70 based on distance matrices, Chem. Phys. Lett. **239** (1995) 117–123.

[10] K. Balasubramanian, Computer generation of distance polynomials of graphs, J. Comput. Chem. **11** (1990) 829–836.

[11] B. Zhou, N. Trinajstić, On the largest eigenvalue of the distance matrix of a connected graph, Chem. Phys. Lett. **447** (2007) 384–387.

[12] B. Zhou, On the largest eigenvalue of the distance matrix of a tree, MATCH Commun. Math. Comput. Chem. **58** (2007) 657–662.

[13] G. Indulal, I. Gutman, On the distance spectra of some graphs, MATCH Commun. Math. Comput. Chem. **13** (2008) 123–131.

[14] G. Indulal, Sharp bounds on the distance spectral radius and the distance energy of graphs, Linear Algebra Appl. **430** (2009) 106–113.

[15] F. R. Gantmacher, The Theory of Matrices, Volume Two, Chelsea Publishing Company, New York, N.Y., 1974.