

Available online at www.sciencedirect.com



LINEAR ALGEBRA AND ITS APPLICATIONS

Linear Algebra and its Applications 428 (2008) 754-764

www.elsevier.com/locate/laa

New upper bounds on the spectral radius of unicyclic graphs $\stackrel{\mbox{\tiny{\sc b}}}{\to}$

Oscar Rojo *,1

Departamento de Matemáticas, Universidad Católica del Norte, Antofagasta, Chile

Received 25 May 2007; accepted 6 August 2007 Available online 29 September 2007 Submitted by R.A. Brualdi

Abstract

Let $\mathscr{G} = (V(\mathscr{G}), E(\mathscr{G}))$ be a unicyclic simple undirected graph with largest vertex degree \varDelta . Let \mathscr{C}_r be the unique cycle of \mathscr{G} . The graph $\mathscr{G} - E(\mathscr{C}_r)$ is a forest of *r* rooted trees $\mathscr{T}_1, \mathscr{T}_2, \ldots, \mathscr{T}_r$ with root vertices v_1, v_2, \ldots, v_r , respectively. Let

 $k(\mathcal{G}) = \max_{1 \leq i \leq r} \{ \max\{ \operatorname{dist}(v_i, u) : u \in V(\mathcal{T}_i) \} \} + 1,$

where dist(v, u) is the distance from v to u. Let $\mu_1(\mathcal{G})$ and $\lambda_1(\mathcal{G})$ be the spectral radius of the Laplacian matrix and adjacency matrix of \mathcal{G} , respectively. We prove that

$$\mu_1(\mathscr{G}) < \varDelta + 2\sqrt{\varDelta - 1} \cos \frac{\pi}{2k(\mathscr{G}) + 1}$$

whenever $\Delta > 2$ and

$$\lambda_1(\mathscr{G}) < 2\sqrt{\varDelta - 1}\cos\frac{\pi}{2k(\mathscr{G}) + 1},$$

whenever $\Delta \ge 4$ or whenever $\Delta = 3$ and $k(\mathscr{G}) \ge 4$. © 2007 Elsevier Inc. All rights reserved.

AMS classification: 5C50; 15A48; 05C05

Keywords: Tree; Unicyclic graph; Laplacian matrix; Adjacency matrix; Spectral radius

0024-3795/\$ - see front matter $_{\odot}$ 2007 Elsevier Inc. All rights reserved. doi:10.1016/j.laa.2007.08.005

^{*} Work supported by Project Fondecyt 1070537, Chile.

^{*} Fax: +56 55 355599.

E-mail address: orojo@ucn.cl

¹ This research was conducted while the author was visitor at the Centro de Modelamiento Matemático, Universidad de Chile, Santiago, Chile.

1. Introduction

Let $\mathscr{G} = (V(\mathscr{G}), E(\mathscr{G}))$ be a simple undirected graph. Let $A(\mathscr{G})$ be the adjacency matrix of \mathscr{G} and let $D(\mathscr{G})$ be the diagonal matrix of vertex degrees. The Laplacian matrix of \mathscr{G} is the matrix $L(\mathscr{G}) = D(\mathscr{G}) - A(\mathscr{G})$. Both $A(\mathscr{G})$ and $L(\mathscr{G})$ are real symmetric matrices. Moreover, $L(\mathscr{G})$ is a positive semidefinite matrix and $(0, \mathbf{e})$ is an eigenpair of $L(\mathscr{G})$, where \mathbf{e} is the all ones vector.

Let $\mu_1(\mathscr{G})$ and $\lambda_1(\mathscr{G})$ be the spectral radius of $L(\mathscr{G})$ and $A(\mathscr{G})$, respectively. It is known that if \mathscr{H} is a subgraph of \mathscr{G} then $\mu_1(\mathscr{H}) \leq \mu_1(\mathscr{G})$ and $\lambda_1(\mathscr{H}) \leq \lambda_1(\mathscr{G})$.

We recall that the distance $dist(u, v), u, v \in V(\mathcal{G})$, is the length of the shortest path in \mathcal{G} from u to v and that the degree $d(v), v \in V(\mathcal{G})$, is the number of edges in $E(\mathcal{G})$ that are incident with v.

Let

$$\Delta = \max\{d(v) : v \in V(\mathscr{G})\}.$$

A tree is a connected acyclic graph. In [6, 2003], Stevanović proves that for a tree \mathcal{T} with largest vertex degree Δ ,

$$\mu_1(\mathscr{T}) < \varDelta + 2\sqrt{\varDelta - 1}$$

and

 $\lambda_1(\mathcal{T}) < 2\sqrt{\Delta - 1}.$

In [2, 2007], Hu proves that if \mathscr{G} is a unicyclic graph then

$$\mu_1(\mathscr{G}) \leqslant \varDelta + 2\sqrt{\varDelta - 1}$$

with equality if and only if \mathscr{G} is the cycle \mathscr{C}_n whenever *n* is even, and

 $\lambda_1(\mathscr{G}) \leqslant 2\sqrt{\varDelta - 1}$

with equality if and only if \mathscr{G} is the cycle \mathscr{C}_n .

From now on, let \mathscr{G} be a unicyclic graph with largest vertex degree $\varDelta > 2$. Let \mathscr{C}_r be the unique cycle of \mathscr{G} and let v_1, v_2, \ldots, v_r be the vertices of \mathscr{C}_r . Then, the graph $\mathscr{G} - E(\mathscr{C}_r)$ is a forest of r rooted trees $\mathscr{T}_1, \mathscr{T}_2, \ldots, \mathscr{T}_r$ with root vertices v_1, v_2, \ldots, v_r , respectively.

Definition 1. For $i = 1, 2, \ldots, r$, we define

$$k_i = \max\{\operatorname{dist}(v_i, u) : u \in V(\mathcal{T}_i)\} + 1$$

and

$$k(\mathscr{G}) = \max\{k_i : 1 \leq i \leq r\}.$$

Let us illustrate this definition with the following example.



For this graph, $\Delta = 5$,

$$\begin{split} k_1 &= \max\{d(v_1, u) : u \in V(\mathcal{F}_1)\} + 1 = 4 + 1 = 5, \\ k_2 &= \max\{d(v_2, u) : u \in V(\mathcal{F}_2)\} + 1 = 3 + 1 = 4, \\ k_3 &= \max\{d(v_3, u) : u \in V(\mathcal{F}_3)\} + 1 = 2 + 1 = 3. \end{split}$$

Then $k(\mathcal{G}) = \max\{5, 4, 3\} = 5.$

In this paper, we derive the new upper bounds

$$\mu_1(\mathscr{G}) < \varDelta + 2\sqrt{\varDelta - 1} \cos \frac{\pi}{2k(\mathscr{G}) + 1},$$

whenever $\Delta > 2$, and

$$\lambda_1(\mathscr{G}) < 2\sqrt{\varDelta - 1}\cos\frac{\pi}{2k(\mathscr{G}) + 1}$$

whenever $\Delta \ge 4$ or whenever $\Delta = 3$ and $k(\mathscr{G}) \ge 4$.

2. Finding the new upper bounds

We begin this section by recalling some results from [4, 2007] that will play an important role in this paper.

The level of a vertex in a rooted tree is one more than its distance from the root vertex. A tree \mathscr{B}_k of k levels is a generalized Bethe tree [4] if vertices at the same level have equal degree. Let \mathscr{B}_k be a generalized Bethe tree of k levels. Let $\mathscr{B}_k^{(r)}$ be the unicyclic graph obtained from the union of r copies of \mathscr{B}_k and the cycle \mathscr{C}_r connecting the r root vertices. We may consider $\mathscr{B}_k^{(r)}$ as a graph of k > 1 levels in which vertices at the same level have equal degree. We agree that the vertices of \mathscr{C}_r are at the level 1. An example of a such graph is

756

Example 1. Let *G* be the graph





This graph has four levels of vertices in which the vertex degree sequence, from the pendant vertices to the vertices in \mathscr{C}_3 , is (1, 3, 4, 4).

For the graph $\mathscr{B}_k^{(r)}$ with k > 1, let d_{k-j+1} be the degree of the vertices at the level j (j = 1, 2, ..., k). Thus, d_k is the degree of the vertices at the level 1, and $d_1 = 1$ is the degree of the vertices at the level k (pendant vertices). Let

$$\mathbf{d} = (1, d_2, \ldots, d_k).$$

As usual, let $\rho(M)$ denotes the spectral radius of the matrix M.

In [4], we characterize completely the spectra of the adjacency matrix and Laplacian matrix of $\mathscr{B}_{k}^{(r)}$. In particular, we derive results concerning $\mu_{1}(\mathscr{B}_{k}^{(r)})$ and $\lambda_{1}(\mathscr{B}_{k}^{(r)})$, which we give in the following lemmas.

Lemma 1 [4, Theorem 3, part (c)]. Let r = 2s or r = 2s + 1. Let $L_{k,s}(\mathbf{d})$ be the $k \times k$ symmetric tridiagonal matrix

$$L_{k,s}(\mathbf{d}) = \begin{bmatrix} 1 & \sqrt{d_2 - 1} & & & \\ \sqrt{d_2 - 1} & d_2 & \sqrt{d_3 - 1} & & \\ & \sqrt{d_3 - 1} & \ddots & \ddots & \\ & & \ddots & d_{k-1} & \sqrt{d_k - 2} \\ & & & \sqrt{d_k - 2} & d_k - 2\cos\frac{2\pi s}{r} \end{bmatrix}$$

Then $\rho(L_{k,s}(\mathbf{d})) = \mu_1(\mathscr{B}_k^{(r)}).$

Lemma 2 [4, Theorem 7, part (d)]. Let $A_{k,0}(\mathbf{d})$ be the $k \times k$ symmetric tridiagonal matrix

$$A_{k,0}(\mathbf{d}) = \begin{bmatrix} 0 & \sqrt{d_2 - 1} & & & \\ \sqrt{d_2 - 1} & 0 & \sqrt{d_3 - 1} & & \\ & \sqrt{d_3 - 1} & \ddots & \ddots & \\ & & \ddots & 0 & \sqrt{d_k - 2} \\ & & & \sqrt{d_k - 2} & 2 \end{bmatrix}$$

Then $\rho(A_{k,0}(\mathbf{d})) = \lambda_1(\mathscr{B}_k^{(r)}).$

Keep in mind that \mathscr{G} is a unicyclic graph with largest vertex degree $\Delta > 2$, in which \mathscr{C}_r is the unique cycle of \mathscr{G} and that $k(\mathscr{G})$ is as in definition 1. For brevity, we write k instead of $k(\mathscr{G})$. Let $\mathscr{B}_k(\Delta)$ be the generalized Bethe tree with vertex degree sequence

 $(1, \Delta, \Delta, \ldots, \Delta, \Delta-2),$

from the pendant vertices to the root vertex. Then, each tree \mathscr{T}_i is an induced subgraph of $\mathscr{B}_k(\Delta)$. Let $\mathscr{B}_k^{(r)}(\Delta)$ be the unicyclic graph obtained from r copies of $\mathscr{B}_k(\Delta)$ and the cycle \mathscr{C}_r connecting the r root vertices. Therefore, \mathscr{G} is an induced subgraph of $\mathscr{B}_k^{(r)}(\Delta)$. Consequently $\mu_1(\mathscr{G}) \leq \mu_1(\mathscr{B}_k^{(r)}(\Delta))$ and $\lambda_1(\mathscr{G}) \leq \lambda_1(\mathscr{B}_k^{(r)}(\Delta))$.

Observe that the vertex degree sequence for $\mathscr{B}_{k}^{(r)}(\varDelta)$ is

 $\mathbf{d} = (1, \varDelta, \varDelta, \ldots, \varDelta, \varDelta).$

We apply Lemma 1 to the graph $\mathscr{B}_{k}^{(r)}(\Delta)$ to get that the spectral radius of the $k \times k$ matrix

is equal to $\mu_1(\mathscr{B}_k^{(r)}(\varDelta))$ and that the spectral radius of the $k \times k$ matrix

$$A_{k,0}(\Delta) = \begin{bmatrix} 0 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 1} & & \\ & \sqrt{\Delta - 1} & \ddots & \ddots & \\ & & \ddots & 0 & \sqrt{\Delta - 2} \\ & & & & \sqrt{\Delta - 2} & 2 \end{bmatrix}$$

is equal to $\lambda_1(\mathscr{B}_k^{(r)}(\varDelta))$.

Therefore in order to find upper bounds on $\mu_1(\mathscr{G})$ and $\lambda_1(\mathscr{G})$, we search for upper bounds on $\rho(L_{k,s}(\Delta))$ and $\rho(A_{k,0}(\Delta))$, respectively.

We recall the following result concerning the spectral radius of a special symmetric tridiagonal matrix.

Lemma 3 [3]. The spectral radius of the $m \times m$ symmetric tridiagonal matrix

$$D_m(b) = \begin{bmatrix} 0 & b & & & \\ b & 0 & b & & \\ & b & \ddots & & \\ & b & \ddots & b & \\ & & b & 0 & b \\ & & & b & b \end{bmatrix}, \quad b > 0$$
(1)

is

$$\rho(D_m(b)) = 2b\cos\frac{\pi}{2m+1}.$$

Theorem 4. Let \mathscr{G} be a unicyclic graph with largest vertex degree $\Delta > 2$. Let $k(\mathscr{G})$ as in definition 1. Then

$$\mu_1(\mathscr{G}) < \varDelta + 2\sqrt{\varDelta - 1} \cos \frac{\pi}{2k(\mathscr{G}) + 1}.$$
(2)

Proof. We know that $\mu_1(\mathscr{G}) \leq \mu_1(\mathscr{B}_k^{(r)}(\varDelta)) = \rho(L_{k,s}(\varDelta))$. We have

$$L_{k,s}(\Delta) = \begin{bmatrix} 1 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & \Delta & \sqrt{\Delta - 1} & & \\ & \sqrt{\Delta - 1} & \ddots & \ddots & \\ & & \ddots & \Delta & \sqrt{\Delta - 2} \\ & & & \sqrt{\Delta - 2} & \Delta - 2\cos\frac{2\pi s}{r} \end{bmatrix}$$
$$\leqslant \begin{bmatrix} 1 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & \Delta & \sqrt{\Delta - 1} & & \\ & \sqrt{\Delta - 1} & \ddots & \ddots & \\ & & \ddots & \Delta & \sqrt{\Delta - 2} \\ & & & & \ddots & \Delta & \sqrt{\Delta - 2} \\ & & & & \sqrt{\Delta - 2} & \Delta + 2 \end{bmatrix} = E_k.$$

Since the spectral radius of an irreducible nonnegative matrix increases when any of its entries increases [8], we have

$$\rho(L_{k,s}(\Delta)) \leqslant \rho(E_k). \tag{3}$$

The matrix E_k has the LL^T -decomposition

$$E_k = LL^T,$$

where L is the lower bidiagonal matrix

$$L = \begin{bmatrix} \frac{1}{\sqrt{d-1}} & 1 & & \\ & \sqrt{d-1} & \ddots & \\ & & \ddots & 1 \\ & & & \sqrt{d-2} & 2 \end{bmatrix}.$$

Then E_k is a positive definite and the matrices $E_k = LL^T$ and $\widetilde{E_k} = L^T L$ have the same eigenvalues [9]. From this fact and (3), we obtain

$$\rho(L_{k,s}(\Delta)) \leqslant \rho(\widetilde{E}_k). \tag{4}$$

.

Computing the product $L^T L$, we obtain

We have

$$\widetilde{E_k} = \operatorname{diag}\{\Delta, \Delta, \dots, \Delta\} + \begin{bmatrix} 0 & \sqrt{\Delta - 1} \\ \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 1} \\ & \sqrt{\Delta - 1} & \ddots & \ddots \\ & & \ddots & -1 & 2\sqrt{\Delta - 2} \\ & & & 2\sqrt{\Delta - 2} & 4 - \Delta \end{bmatrix}$$

$$= \operatorname{diag}\{\varDelta, \varDelta, \ldots, \varDelta\} + F_k,$$

where

$$F_{k} = \begin{bmatrix} 0 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 1} & & \\ & \sqrt{\Delta - 1} & \ddots & \ddots & \\ & & \ddots & & \ddots & \\ & & & \ddots & & -1 & 2\sqrt{\Delta - 2} \\ & & & & 2\sqrt{\Delta - 2} & 4 - \Delta \end{bmatrix}.$$

From (1),

$$D_k(\sqrt{\Delta - 1}) = \begin{bmatrix} 0 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 1} & & \\ & \sqrt{\Delta - 1} & \ddots & \ddots & \\ & & \ddots & 0 & \sqrt{\Delta - 1} \\ & & & \sqrt{\Delta - 1} & \sqrt{\Delta - 1} \end{bmatrix}.$$

We define

$$\begin{aligned} G_k &= D_k (\sqrt{\Delta - 1}) - F_k \\ &= \begin{bmatrix} 0 & 0 & & & \\ 0 & \ddots & \ddots & & \\ & \ddots & 0 & 0 & \\ & & 0 & 1 & \sqrt{\Delta - 1} - 2\sqrt{\Delta - 2} \\ & & & \sqrt{\Delta - 1} - 2\sqrt{\Delta - 2} & \sqrt{\Delta - 1} - 4 + \Delta \end{bmatrix}. \end{aligned}$$

760

Since $\Delta \ge 3$, one can prove that the submatrix

$$\begin{bmatrix} 1 & \sqrt{\varDelta - 1} - 2\sqrt{\varDelta - 2} \\ \sqrt{\varDelta - 1} - 2\sqrt{\varDelta - 2} & -4 + \varDelta + \sqrt{\varDelta - 1} \end{bmatrix}$$

is a positive definite matrix. Hence G_k is positive semidefinite matrix. Since F_k is an irreducible nonnegative matrix, there exists unitary eigenvector $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1^T & \mathbf{x}_2^T \end{bmatrix} > \mathbf{0}$ such that $\mathbf{x}^T F_k \mathbf{x} = \rho(F_k)$ [8]. Therefore $\mathbf{x}_2 \neq \mathbf{0}$ and

$$\mathbf{x}^{T} D_{k}(\sqrt{\Delta - 1})\mathbf{x} = \mathbf{x}^{T} F_{k}\mathbf{x} + \mathbf{x}^{T} G_{k}\mathbf{x}$$

$$= \rho(F_{k})$$

$$+ \mathbf{x}_{2}^{T} \begin{bmatrix} 1 & \sqrt{\Delta - 1} - 2\sqrt{\Delta - 2} \\ \sqrt{\Delta - 1} - 2\sqrt{\Delta - 2} & -4 + \Delta + \sqrt{\Delta - 1} \end{bmatrix} \mathbf{x}_{2}$$

$$> \rho(F_{k}).$$

Then

$$\rho(F_k) < \mathbf{x}^T D_k(\sqrt{\Delta - 1}) \mathbf{x} \leqslant \rho(D_k(\sqrt{\Delta - 1})).$$

From Lemma 3, the spectral radius of $D_{k-1}(\sqrt{\Delta-1})$ is

$$\rho(D_k(\sqrt{\Delta-1})) = 2\sqrt{\Delta-1}\cos\frac{\pi}{2k+1}.$$

Therefore

$$\rho(F_k) < 2\sqrt{\Delta - 1} \cos \frac{\pi}{2k + 1}.$$

Consequently

$$\lambda_1(\widetilde{E}_k) = \varDelta + \lambda_1(F_k)$$

$$< \varDelta + 2\sqrt{\varDelta - 1} \cos \frac{\pi}{2k + 1}.$$
(5)

From (4) and (5), we get

$$\rho(L_{k,s}(\Delta)) < \Delta + 2\sqrt{\Delta - 1} \cos \frac{\pi}{2k + 1}.$$

Since $\mu_1(\mathscr{G}) \leq \mu_1(\mathscr{B}_k^{(r)}) = \rho(L_{k,s}(\varDelta))$ and $k = k(\mathscr{G})$, the upper bound (2) is proved. \Box

At this point, it is convenient to recall some other known results on symmetric tridiagonal matrices [1,5,7].

Lemma 5. 1. The characteristic polynomials, $q_j(\lambda)$, of the $j \times j$ leading principal submatrix of the $k \times k$ symmetric tridiagonal matrix

$$Q_{k} = \begin{bmatrix} a_{1} & b_{1} & & & \\ b_{1} & a_{2} & b_{2} & & & \\ & b_{2} & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & a_{k-1} & b_{k-1} \\ & & & & b_{k-1} & a_{k} \end{bmatrix}$$
(6)

satisfy the three-term recursion formula

$$q_j(\lambda) = (\lambda - a_j)q_{j-1}(\lambda) - b_{j-1}^2 q_{j-2}(\lambda)$$

with $q_0(\lambda) = 1$ and $q_1(\lambda) = \lambda - a_1$.

2. If all codiagonal entries b_i (i = 1, 2, ..., k - 1) in (6) are nonzero, the recursion polynomial $q_j(j = 0, 1, ..., k)$ has j real simple zeros. For $1 \le j \le k - 1$, they strictly interlace those of q_{j+1} .

Theorem 6. Let \mathscr{G} be a unicyclic graph with largest vertex degree $\Delta > 2$. Let $k(\mathscr{G})$ as in definition 1. Then

$$\lambda_1(\mathscr{G}) < 2\sqrt{\varDelta - 1} \cos \frac{\pi}{2k(\mathscr{G}) + 1},\tag{7}$$

whenever $\Delta \ge 4$ or whenever $\Delta = 3$ and $k(\mathscr{G}) \ge 4$.

Proof. We know that $\lambda_1(\mathscr{G}) \leq \lambda_1(\mathscr{B}_k^{(r)}(\varDelta)) = \rho(A_{k,0}(\varDelta))$. Suppose $\varDelta \geq 5$. Then

$$A_{k,0}(\Delta) = \begin{bmatrix} 0 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 1} & & \\ & \sqrt{\Delta - 1} & \ddots & \ddots & \\ & & \ddots & 0 & \sqrt{\Delta - 2} \\ & & & \sqrt{\Delta - 2} & 2 \end{bmatrix}$$
$$\leqslant \begin{bmatrix} 0 & \sqrt{\Delta - 1} & & & \\ \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 1} & & \\ & \sqrt{\Delta - 1} & \ddots & \ddots & \\ & & & \ddots & 0 & \sqrt{\Delta - 1} \\ & & & & \sqrt{\Delta - 1} & \sqrt{\Delta - 1} \end{bmatrix} = D_k(\sqrt{\Delta - 1})$$

with strict inequality in position (k - 1, k). Therefore

$$\rho(A_{k,0}(\varDelta)) < \rho(D_k(\sqrt{\varDelta - 1})) = 2\sqrt{\varDelta - 1}\cos\frac{\pi}{2k + 1}.$$

Thus the bound (7) is proved for $\Delta \ge 5$. It remains to study the cases $\Delta = 3$ and $\Delta = 4$. For j = 1, 2, ..., k, let $a_j(\lambda)$ and $d_j(\lambda)$ be the characteristic polynomials of the $j \times j$ leading principal submatrices of $A_{k,0}(\Delta)$ and $D_k(\sqrt{\Delta - 1})$, respectively. Observe that $a_j(\lambda)$ and $d_j(\lambda)$ are identical polynomials (j = 1, 2, ..., k - 1), and that $a_k(\lambda)$ and $d_k(\lambda)$ are the characteristic polynomials of $A_{k,0}(\Delta)$ and $D_k(\sqrt{\Delta - 1})$, respectively. From Lemma 5, part 1, we have

$$a_k(\lambda) = (\lambda - 2)a_{k-1}(\lambda) - (\varDelta - 2)a_{k-2}(\lambda)$$
(8)

and

$$d_k(\lambda) = (\lambda - \sqrt{\Delta - 1})a_{k-1}(\lambda) - (\Delta - 1)a_{k-2}(\lambda).$$
(9)

From (8) and (9), we obtain

$$a_k(\lambda) - d_k(\lambda) = (\sqrt{\Delta} - 1 - 2)a_{k-1}(\lambda) + a_{k-2}(\lambda).$$
(10)

From Lemma 5, part 2, we may write

$$a_k(\lambda) = (\lambda - \alpha_1)(\lambda - \alpha_2) \cdots (\lambda - \alpha_{k-1})(\lambda - \alpha_k),$$

where

 $\alpha_k < \alpha_{k-1} < \cdots < \alpha_2 < \alpha_1$

are the zeros of the polynomial $a_k(\lambda)$. Let $\Delta = \rho(D_k(\sqrt{\Delta - 1}))$. Then, Δ is the largest zero of $d_k(\lambda)$. Since, from Lemma 3,

$$\Delta = 2\sqrt{\Delta - 1}\cos\frac{\pi}{2k + 1},$$

to show (7) it is sufficient to prove that $\Delta > \alpha_1$. Let β_1 be the largest zero of the identical polynomials $d_{k-1}(\lambda)$ and $a_{k-1}(\lambda)$. Since the zeros of these polynomials strictly interlace the zeros of the polynomials $a_k(\lambda)$ and $d_k(\lambda)$, we obtain that $\alpha_2 < \beta_1 < \alpha_1$ and $\beta_1 < \Delta$. Therefore $\alpha_2 < \Delta$, $a_{k-1}(\Delta) > 0$ and

$$a_k(\Delta) = (\Delta - \alpha_1)(\Delta - \alpha_2) \cdots (\Delta - \alpha_{k-1})(\Delta - \alpha_k)$$

= $(\Delta - \alpha_1)P$,

where P > 0. Thus, to show that $\Delta > \alpha_1$ it is sufficient to prove that $a_k(\Delta) > 0$. From (9) and (10),

$$(\varDelta - \sqrt{\varDelta - 1})a_{k-1}(\varDelta) - (\varDelta - 1)a_{k-2}(\varDelta) = 0$$

and

$$a_k(\Delta) = (\sqrt{\Delta - 1} - 2)a_{k-1}(\Delta) + a_{k-2}(\Delta).$$

Then

$$a_k(\varDelta) = \left(\sqrt{\varDelta - 1} - 2 + \frac{\varDelta - \sqrt{\varDelta - 1}}{\varDelta - 1}\right) a_{k-1}(\varDelta).$$
(11)

Let $\Delta = 4$. From (11)

$$a_{k}(\varDelta) = \left(\sqrt{3} - 2 + \frac{2\sqrt{3}\cos\frac{\pi}{2k+1} - \sqrt{3}}{3}\right)a_{k-1}(\varDelta)$$
$$= \left(\frac{2\sqrt{3}}{3} - 2 + \frac{2\sqrt{3}}{3}\cos\frac{\pi}{2k+1}\right)a_{k-1}(\varDelta)$$
$$\geqslant \left(\frac{2\sqrt{3}}{3} - 2 + \frac{2\sqrt{3}}{3}\cos\frac{\pi}{5}\right)a_{k-1}(\varDelta)$$
$$> 0.08a_{k-1}(\varDelta) > 0.$$

Let now $\Delta = 3$ and $k \ge 4$. From (11)

$$a_{k}(\varDelta) = \left(\sqrt{2} - 2 + \frac{2\sqrt{2}\cos\frac{\pi}{2k+1} - \sqrt{2}}{2}\right)a_{k-1}(\varDelta)$$
$$= \left(\frac{\sqrt{2}}{2} - 2 + \sqrt{2}\cos\frac{\pi}{2k+1}\right)a_{k-1}(\varDelta)$$

$$\geq \left(\frac{\sqrt{2}}{2} - 2 + \sqrt{2}\cos\frac{\pi}{9}\right) a_{k-1}(\varDelta)$$
$$> 0.03a_{k-1}(\varDelta) > 0.$$

The proof is complete. \Box

Remark 1. The bound (7) does not hold for $\Delta = 3$ if $k(\mathcal{G}) = 2$ or $k(\mathcal{G}) = 3$. In fact, to four decimal places, the spectral radius of

$$A_{2,0}(3) = \begin{bmatrix} 0 & 1\\ 1 & 2 \end{bmatrix}$$

is 2.4142 and $2\sqrt{2}\cos\frac{\pi}{5} = 2.2882$, and the spectral radius of

$$A_{3,0}(3) = \begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

is 2.5616 and $2\sqrt{2}\cos\frac{\pi}{7} = 2.5483$.

Acknowledgments

The author wishes to thank the referee for the valuable comments which led to an improved version of the paper.

References

- [1] G.H. Golub, C.F. Van Loan, Matrix Computations, second ed., Johns Hopkins University Press, Baltimore, 1989.
- [2] S. Hu, The largest eigenvalue of unicyclic graphs, Discrete Math. 307 (2007) 280-284.
- [3] S. Kouachi, Eigenvalues and eigenvectors of tridiagonal matrices, Electron. J. Linear Algebra 15 (April) (2006) 115–133.
- [4] O. Rojo, The spectra of a graph obtained from copies of a generalized Bethe tree, Linear Algebra Appl. 420 (2–3) (2007) 490–507.
- [5] H.R. Schwarz, H. Rutishauser, E. Stiefel, Numerical Analysis of Symmetric Matrices, Prentice-Hall, 1973.
- [6] D. Stevanović, Bounding the largest eigenvalue of trees in terms of the largest vertex degree, Linear Algebra Appl. 360 (2003) 35–42.
- [7] L.N. Trefethen, D. Bau III, Numerical Linear Algebra, Society for Industrial and Applied Mathematics, 1997.
- [8] R.S. Varga, Matrix Iterative Analysis, Prentice-Hall, 1965.
- [9] F. Zhang, Matrix Theory, Springer, 1999.

764