A\textsubscript{\(\alpha\)}-spectrum of a graph obtained by copies of a rooted graph and applications

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Abstract

Given a connected graph \(R\) on \(r\) vertices and a rooted graph \(H\), let \(R\{H\}\) be the graph obtained from \(r\) copies of \(H\) and the graph \(R\) by identifying the root of the \(i\)th copy of \(H\) with the \(i\)th vertex of \(R\). Let \(0 \leq \alpha \leq 1\), and let

\[
A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)
\]

where \(D(G)\) and \(A(G)\) are the diagonal matrix of the vertex degrees of \(G\) and the adjacency matrix of \(G\), respectively. A basic result on the \(A_\alpha\)-spectrum of \(R\{H\}\) is obtained. This result is used to prove that if \(H = B_k\) is a generalized Bethe tree on \(k\) levels, then the eigenvalues of \(A_\alpha(R\{B_k\})\) are the eigenvalues of symmetric tridiagonal matrices of order not exceeding \(k\); additionally, the multiplicity of each eigenvalue is determined. Finally, applications to a unicyclic graph are given, including an upper bound on the \(\alpha\)-spectral radius in terms of the largest vertex degree and the largest height of the trees obtained by removing the edges of the unique cycle in the graph.

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1 Introduction

Let \(G = (V(G), E(G))\) be a simple undirected graph on \(n\) vertices with vertex set \(V(G)\) and edge set \(E(G)\). Let \(D(G)\) be the diagonal matrix of order \(n\) whose \((i, i)\)–entry is the degree of the \(i\)th vertex of \(G\) and let \(A(G)\) be the adjacency matrix of \(G\). The matrices \(L(G) = D(G) - A(G)\) and \(Q(G) = D(G) + A(G)\) are the Laplacian and signless Laplacian matrix of \(G\), respectively. The matrices \(L(G)\) and \(Q(G)\) are both positive semidefinite and \((0, 1)\) is an eigenpair of \(L(G)\) where \(1\) is the all ones vector. For a connected graph \(G\), the smallest eigenvalue of \(Q(G)\) is positive if and only if \(G\) is non-bipartite.

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In [7], the family of matrices $A_\alpha(G)$,

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$$

with $\alpha \in [0,1]$, is introduced together with a number of some basic results and several open problems.

Observe that $A_0(G) = A(G)$ and $A_{1/2}(G) = \frac{1}{2}Q(G)$.

Let $R$ be a connected graph on $r$ vertices. Let $v_1, \ldots, v_r$ be the vertices of $R$. Let $\epsilon_{ij} = \epsilon_{ji} = 1$ if $v_i \sim v_j$ and let $\epsilon_{ij} = \epsilon_{ji} = 0$ otherwise.

We recall that a rooted graph is a graph in which one vertex has been distinguished as the root and that the level of a vertex is one more than its distance from the root. In particular, a generalized Bethe tree is a rooted tree in which vertices at the same level have the same degree.

Let $H$ be a rooted graph. Let $R\{H\}$ be the graph obtained from $R$ and $r$ copies of $H$ by identifying the root of the $i-$copy of $H$ with the vertex $v_i$ of $R$.

In this paper, we obtain a general result on the $A_\alpha-$ spectrum of $R\{H\}$. We use this result to prove that if $H = B_k$ is a generalized Bethe tree on $k$ levels, then the eigenvalues of $A_\alpha (R\{B_k\})$ are the eigenvalues of symmetric tridiagonal matrices of order not exceeding $k$; additionally, the multiplicity of each eigenvalue is determined. Finally, we apply these results to a unicyclic graph, including the derivation of an upper bound on the $\alpha-$ spectral radius in terms of the largest vertex degree and the largest height of the trees obtained by removing the edges of the unique cycle in the graph.

## 2 A basic result on the $A_\alpha-$ spectrum of copies of a rooted graph

Let $E$ be the matrix of order $n \times n$ with 1 in the $(n,n)$–entry and zeros elsewhere. For $i = 1, 2, \ldots, r$, let $d(v_i)$ be the degree of $v_i$ as a vertex of $R$ and let $n$ be the order of $H$. Then the total number of vertices in $R\{H\}$ is $rn$. We label the vertices of $R\{H\}$ as follows: for $i = 1, 2, \ldots, r$, using the labels $(i-1)n+1, (i-1)n+2, \ldots, in$, we label the vertices of the $i-$th copy of $H$ from the vertices at the bottom (the set of vertices at the largest distance from the root) to the vertex $v_i$.

From now on, let $\alpha \in [0,1]$ and let $\beta = 1 - \alpha$. With the above labeling, we obtain $A_\alpha (R\{H\}) =$

\[
\begin{bmatrix}
A_\alpha(H) + \alpha d(v_1)E & \beta_1E & \cdots & \cdots & \beta rE \\
\beta_1E & \ddots & \ddots & & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\beta_1E & \beta_2E & \cdots & \beta rE & A_\alpha(H) + \alpha d(v_r)E
\end{bmatrix}
\]

(1)

In this paper, the identity matrix of appropriate order is denoted by $I$ and $I_m$ denotes the identity matrix of order $m$. Furthermore, we need the following additional notation: $|M|$ and
\( \phi_M(\lambda) \) denote the determinant and the characteristic polynomial of \( M \), respectively, and \( B^T \) denotes the transpose of \( B \).

The Kronecker product \([12]\) of two matrices \( A = (a_{ij}) \) and \( B = (b_{ij}) \) of sizes \( m \times m \) and \( n \times n \), respectively, is the \((mn) \times (mn)\) matrix \( A \otimes B = (a_{ij}B) \). Then, in particular, \( I_n \otimes I_m = I_{nm} \). Some basic properties of the Kronecker product are \((A \otimes B)^T = A^T \otimes B^T\) and \((A \otimes B) (C \otimes D) = AC \otimes BD\) for matrices of appropriate sizes. Moreover, if \( A \) and \( B \) are invertible matrices then \( (A \otimes B)^{-1} = A^{-1} \otimes B^{-1} \).

Let \( \text{Spec}(M) \) be the spectrum of a matrix \( M \).

**Theorem 1** Let \( \rho_1(\alpha), \rho_2(\alpha), \ldots, \rho_r(\alpha) \) be the eigenvalues of \( A_\alpha(R) \). Then

\[
\text{Spec}(A_\alpha(R\{H\})) = \bigcup_{j=1}^r \text{Spec}(A_\alpha(H) + \rho_j(\alpha)E). \tag{2}
\]

**Proof** From (1)

\[
A_\alpha(R\{H\}) = I_r \otimes A_\alpha(H) + A_\alpha(R) \otimes E.
\]

Let

\[
V = \begin{bmatrix} v_1 & v_2 & \cdots & v_{r-1} & v_r \end{bmatrix}
\]

be an orthogonal matrix whose columns \( v_1, v_2, \ldots, v_r \) are eigenvectors corresponding to the eigenvalues \( \rho_1(\alpha), \rho_2(\alpha), \ldots, \rho_r(\alpha) \), respectively. Then

\[
(V \otimes I_n)A_\alpha(R\{H\})(V^T \otimes I_n) = (V \otimes I_n)(I_r \otimes A_\alpha(H) + A_\alpha(R) \otimes E)(V^T \otimes I_n)
\]

\[
= I_r \otimes A_\alpha(H) + (VA_\alpha(R)V^T) \otimes E.
\]

Moreover,

\[
(VA_\alpha(R)V^T) \otimes E = \begin{bmatrix} \rho_1(\alpha) & & \\ & \rho_2(\alpha) & \\ & & \ddots \end{bmatrix} \otimes E
\]

\[
= \begin{bmatrix} \rho_1(\alpha)E & & \\ & \rho_2(\alpha)E & \\ & & \ddots \end{bmatrix}.
\]
Therefore,

\[(V \otimes I_n)A_\alpha(R\{H\})(V^T \otimes I_n) = \begin{bmatrix}
A_\alpha(H) + \rho_1(\alpha)E & A_\alpha(H) + \rho_2(\alpha)E & \cdots & A_\alpha(H) + \rho_r(\alpha)E \\
A_\alpha(H) + \rho_1(\alpha)E & A_\alpha(H) + \rho_2(\alpha)E & \cdots & A_\alpha(H) + \rho_r(\alpha)E \\
\vdots & \vdots & \ddots & \vdots \\
A_\alpha(H) + \rho_1(\alpha)E & A_\alpha(H) + \rho_2(\alpha)E & \cdots & A_\alpha(H) + \rho_r(\alpha)E
\end{bmatrix}.
\]

Since \(A_\alpha(R\{H\})\) and \((V \otimes I_n)A_\alpha(R\{H\})(V^T \otimes I_n)\) are similar matrices, (2) follows. \(\square\)

3 \(A_\alpha\)-spectrum of copies of a generalized Bethe tree

From now on, let \(B_k\) be a generalized Bethe tree of \(k\) levels. From Theorem 1, we have

**Theorem 2** Let \(\rho_1(\alpha), \rho_2(\alpha), \ldots, \rho_r(\alpha)\) be the eigenvalues of \(A_\alpha(R)\). Then

\[\text{Spec}(A_\alpha(R\{B_k\})) = \bigcup_{i=1}^r \text{Spec}(A_\alpha(B_k) + \rho_i(\alpha)E).\]

For \(1 \leq j \leq k\), let \(n_j\) and \(d_j\) be the number and the degree of the vertices of \(B_k\) at the level \(k - j + 1\), respectively. Thus \(d_k\) is the degree of the root, \(n_k = 1\), \(d_1 = 1\) and \(n_1\) is the number of pendant vertices. For \(1 \leq j \leq k - 1\), let \(m_j = \frac{n_j}{n_{j+1}}\).

**Definition 3** Let

\[P_0(\lambda) = 1, \quad P_1(\lambda) = \lambda - \alpha,\]

and

\[P_j(\lambda) = (\lambda - ad_j)P_{j-1}(\lambda) - \beta^2 m_{j-1}P_{j-2}(\lambda)\]

for \(j = 2, \ldots, k\).

For brevity, sometimes we write \(f\) instead \(f(\lambda)\). The polynomials in Definition 3 are used in [8], Theorem 5, to factor the characteristic polynomial of \(A_\alpha(B_k)\) as given below.

**Theorem 4** The characteristic polynomial of \(A_\alpha(B_k)\) satisfies

\[\phi_{A_\alpha(B_k)}(\lambda) = P_1^{n_1-n_2}P_2^{n_2-n_3} \cdots P_{k-2}^{n_{k-2}-n_{k-1}}P_{k-1}^{n_{k-1}-1}P_k.\] (3)

At this point, we introduce the notation \(\tilde{M}\) to mean the matrix obtained from \(M\) by deleting its last row and its last column.

For \(1 \leq i \leq r\), consider the matrices \(A_\alpha(B_k) + \rho_i(\alpha)E\) in Theorem 2. Let

\[M_i(\alpha) = A_\alpha(B_k) + \rho_i(\alpha)E.\]
Then
\[ \phi_{M_i(\alpha)}(\lambda) = |\lambda I - A_\alpha(B_k) - \rho_i(\alpha)E|. \]
Applying linearity on the last column, we obtain
\[ \phi_{M_i(\alpha)}(\lambda) = |\lambda I - A_\alpha(B_k)| - \rho_i(\alpha)|\lambda I - \overline{A_\alpha(B_k)}| = \phi_{A_\alpha(B_k)}(\lambda) - \rho_i(\alpha)\phi_{\overline{A_\alpha(B_k)}}(\lambda). \] (4)

Theorem 4 gives \( \phi_{A_\alpha(B_k)}(\lambda) \) as a product of powers of the polynomials \( P_j(\lambda) \) \((1 \leq j \leq k)\). We now focus our attention on \( \phi_{\overline{A_\alpha(B_k)}}(\lambda) \). From the proof of Theorem 5 in [8], we have
\[ \phi_{A_\alpha(B_k)}(\lambda) = \phi_{\overline{A_\alpha(B_k)}}(\lambda) \frac{P_k}{P_{k-1}}. \]
From this identity and Theorem 4, we obtain
\[ \phi_{\overline{A_\alpha(B_k)}}(\lambda) = P_{n_1-n_2} P_{n_2-n_3} \ldots P_{n_{k-2}-n_{k-1}} P_{n_k} \]
Replacing in (4) and factoring, we get

**Lemma 5** Let \( \rho_1(\alpha), \rho_2(\alpha), \ldots, \rho_r(\alpha) \) be the eigenvalues of \( A_\alpha(R) \). For \( i = 1, \ldots, r \), the characteristic polynomial of \( M_i(\alpha) = A_\alpha(B_k) + \rho_i(\alpha)E \) satisfies
\[ \phi_{M_i(\alpha)}(\lambda) = P_{n_1-n_2} P_{n_2-n_3} \ldots P_{n_{k-2}-n_{k-1}} P_{n_k}(P_k - \rho_i(\alpha)P_{k-1}). \]

**Definition 6** For \( j = 1, 2, \ldots, k-1 \), let \( T_j \) be the \( j \times j \) leading principal submatrix of the \( k \times k \) symmetric tridiagonal matrix
\[
T_k = \begin{bmatrix}
\alpha & \beta \sqrt{d_2-1} & 0 & 0 \\
\beta \sqrt{d_2-1} & ad_2 & \ddots & \\
& \ddots & \ddots & \beta \sqrt{d_{k-1}-1} \\
0 & \beta \sqrt{d_{k-1}-1} & ad_{k-1} & \beta \sqrt{d_k} \\
0 & 0 & \beta \sqrt{d_k} & ad_k
\end{bmatrix}, \quad (5)
\]
Since \( d_s > 1 \) for all \( s = 2, 3, \ldots, j \), each matrix \( T_j \) has nonzero codiagonal entries and it is known that its eigenvalues are simple.

The relationship between these matrices and the polynomials \( P_j(\lambda) \) is given in [8], Lemma 7:

**Lemma 7** For \( j = 1, \ldots, k \),
\[ \phi_{T_j}(\lambda) = P_j(\lambda). \]
Definition 8 For \( i = 1, \ldots, r \), let \( Q_i(\lambda) \) be the polynomial
\[
Q_i(\lambda) = P_k(\lambda) - \rho_i(\alpha)P_{k-1}(\lambda)
\]
and \( S_i \) be the \( k \times k \) matrix
\[
S_i = \begin{bmatrix}
\alpha & \beta\sqrt{d_2-1} & 0 & 0 \\
\beta\sqrt{d_2-1} & \beta d_2 \cdots & \cdots & \beta\sqrt{d_{k-1}-1} \\
& \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \beta\sqrt{d_k-1} - 1 & \beta \sqrt{d_k} & \beta \sqrt{d_k} + \rho_i(\alpha)
\end{bmatrix}.
\]

The relationship between the polynomials \( Q_i \) and the matrices \( S_i \) is given in the following lemma.

Lemma 9 For \( i = 1, \ldots, r \), \( Q_i(\lambda) \) is the characteristic polynomial of the \( k \times k \) matrix \( S_i \), that is,
\[
\phi_{S_i}(\lambda) = Q_i(\lambda).
\]

Proof Applying linearity on the last column, we obtain
\[
\phi_{S_i}(\lambda) = |\lambda I - S_i| = |\lambda I - T_k| - \rho_i(\alpha)|\lambda I - T_{k-1}|.
\]
Now Lemma 7 implies that
\[
\phi_{S_i}(\lambda) = P_k(\lambda) - \rho_i(\alpha)P_{k-1}(\lambda) = Q_i(\lambda).
\]

We are ready to state the main result of this section.

Theorem 10 Let \( B_k \) be a generalized Bethe tree on \( k \) levels, and \( \alpha \in [0, 1) \). Let \( \rho_1(\alpha) \ldots \rho_r(\alpha) \) be the eigenvalues of \( A_\alpha(R) \) in which \( \rho_1(\alpha) \) is the spectral radius. If the matrices \( T_1, \ldots, T_k \) and \( S_1, \ldots, S_r \) are as in Definitions 6 and 8, respectively, then
\[
(1) \quad \text{Spec}(A_\alpha(R\{B_k\})) = (\cup_{j=1}^{k-1}\text{Spec}(T_j)) \cup (\cup_{i=1}^r\text{Spec}(S_i)).
\]

(2) For \( 1 \leq j \leq k - 1 \), the multiplicity of each eigenvalue of \( T_j \) as an eigenvalue of \( A_\alpha(R\{B_k\}) \) is \( r(n_{j} - n_{j+1}) \), and for \( 1 \leq i \leq r \), the eigenvalues of \( S_i \) as eigenvalues of \( A_\alpha(R\{B_k\}) \) are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.

(3) The largest eigenvalue of \( S_1 \) is the spectral radius of \( A_\alpha(R\{B_k\}) \).
Proof (1) and (2) are consequences of Theorem 2, Lemma 5, Lemma 7 and Lemma 9. The eigenvalues of each $T_j$ interlace the eigenvalues of any $S_i$. Then the spectral radius of $A_\alpha(R\{B_k\})$ is the largest of the spectral radii of the matrices $S_i$. We use the fact that the spectral radius of an irreducible nonnegative matrix increases when any of its entries increases, to obtain item (3).

A Bethe tree $B(d,k)$ is a rooted tree of $k$ levels in which the root has degree $d$, the vertices at level $j$ ($2 \leq j \leq k-1$) have degree $d+1$ and the vertices at level $k$ have degree equal to 1 (pendant vertices). Clearly, any Bethe tree is a generalized Bethe tree. Theorem 10 immediately implies the following corollary.

**Corollary 11** Let $\alpha \in [0, 1)$, and $\beta = 1 - \alpha$. Let $\rho_1(\alpha), \ldots, \rho_r(\alpha)$ be the eigenvalues of $A_\alpha(R)$ in which $\rho_1(\alpha)$ is the spectral radius. For $1 \leq j \leq k$, let $T_j$ be the leading principal submatrix of order $j \times j$ of the $k \times k$ symmetric tridiagonal matrix

$$
T_k = \begin{bmatrix}
\alpha & \beta \sqrt{d} & 0 & 0 \\
\beta \sqrt{d} & \alpha (d+1) & \beta \sqrt{d} & \\
& \ddots & \ddots & \ddots \\
0 & 0 & \beta \sqrt{d} & \alpha (d+1) \\
\end{bmatrix}.
$$

For $1 \leq i \leq r$, let

$$
S_i = \begin{bmatrix}
\alpha & \beta \sqrt{d} & 0 & 0 \\
\beta \sqrt{d} & \alpha (d+1) & \beta \sqrt{d} & \\
& \ddots & \ddots & \ddots \\
0 & 0 & \beta \sqrt{d} & \alpha (d+1) + \beta \sqrt{d} \\
\end{bmatrix}.
$$

Then

(1) \quad \text{Spec}(A_\alpha(R\{B(d,k)\})) = (\bigcup_{j=1}^{k-1}\text{Spec}(T_j)) \cup (\bigcup_{i=1}^{r}\text{Spec}(S_i)).

(2) For $1 \leq j \leq k-1$, the multiplicity of each eigenvalue of $T_j$ as an eigenvalue of $A_\alpha(R\{B(d,k)\})$ is $rd^{2j-1}(d-1)$, and for $1 \leq i \leq r$, the eigenvalues of $S_i$ as eigenvalues of $A_\alpha(R\{B(d,k)\})$ are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.

(3) The largest eigenvalue of $S_1$ is the spectral radius of $A_\alpha(R\{B(d,k)\})$.

4 Applications to unicyclic graphs. An upper bound on the $A_\alpha$-spectral radius

In this section we consider $R = C_r$, the cycle on $r$ vertices. It is known that the eigenvalues of the adjacency matrix of $C_r$ are $2 \cos(\frac{2\pi(i-1)}{r})$, $1 \leq i \leq r$. Since the cycle $C_r$ is a 2-regular graph, it
follows that the eigenvalues of \( A_\alpha(C_r) \) are

\[
\rho_i(\alpha) = 2\alpha + 2(1 - \alpha) \cos\left(\frac{2\pi(i - 1)}{r}\right)
\]

for \( i = 1, \ldots, r \). Hence the spectral radius of \( A_\alpha(C_r) \) is \( \rho_1(\alpha) = 2 \) for any \( \alpha \in [0, 1] \).

From Theorem 10, we have

**Corollary 12** Let \( B_k \) be a generalized Bethe tree of \( k \) levels. Let \( T_1, \ldots, T_k \) be as in Definitions 6. For \( i = 1, \ldots, r \), let \( S_i \) be the \( k \times k \) matrix

\[
S_i = \begin{bmatrix}
\alpha & \beta \sqrt{d_2 - 1} & 0 & 0 \\
\beta \sqrt{d_2 - 1} & \alpha d_2 & \ddots & \\
& \ddots & \ddots & \beta \sqrt{d_{k-1} - 1} \\
0 & 0 & \beta \sqrt{d_{k-1}} & \alpha d_k + 2\alpha + 2(1 - \alpha) \cos\left(\frac{2\pi(i - 1)}{r}\right)
\end{bmatrix}.
\]

Then

1. \( \text{Spec}(A_\alpha(C_r\{B_k\})) = (\cup_{j=1}^{k-1}\text{Spec}(T_j)) \cup (\cup_{i=1}^{r}\text{Spec}(S_i)). \) (7)
2. For \( 1 \leq j \leq k - 1 \), the multiplicity of each eigenvalue of \( T_j \) as an eigenvalue of \( A_\alpha(C_r\{B_k\}) \) is \( r(n_j - n_{j+1}) \), and for \( 1 \leq i \leq r \), the eigenvalues of \( S_i \) as eigenvalues of \( A_\alpha(C_r\{B_k\}) \) are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.
3. The largest eigenvalue of

\[
S_1 = \begin{bmatrix}
\alpha & \beta \sqrt{d_2 - 1} & 0 & 0 \\
\beta \sqrt{d_2 - 1} & \alpha d_2 & \ddots & \\
& \ddots & \ddots & \beta \sqrt{d_{k-1} - 1} \\
0 & 0 & \beta \sqrt{d_{k-1}} & \alpha d_k + 2\alpha + 2(1 - \alpha) \cos\left(\frac{2\pi(i - 1)}{r}\right)
\end{bmatrix}
\]

is the spectral radius of \( A_\alpha(C_r\{B_k\}) \).

For the case of copies of the Bethe tree \( B(d, k) \) attached to \( C_r \), from Corollary 11, we have

**Corollary 13** Let \( \alpha \in [0, 1] \), and \( \beta = 1 - \alpha \). For \( 1 \leq j \leq k \), let \( T_j \) be as Corollary 11. For \( 1 \leq i \leq r \), let

\[
S_i = \begin{bmatrix}
\alpha & \beta \sqrt{d} & 0 & 0 \\
\beta \sqrt{d} & \alpha (d + 1) & \beta \sqrt{d} & \ddots \\
& \ddots & \ddots & \alpha (d + 1) \\
0 & 0 & \beta \sqrt{d} & \alpha d + 2\alpha + 2\beta \cos\left(\frac{2\pi(i - 1)}{r}\right)
\end{bmatrix}.
\]
Then

1. The spectrum of $A_\alpha(C_r\{B(d,k)\})$ is the multiset union
   \[
   \text{Spec}(A_\alpha(C_r\{B(d,k)\})) = (\bigcup_{j=1}^{k-1}\text{Spec}(T_j)) \cup (\bigcup_{i=1}^{r}\text{Spec}(S_i)).
   \]

2. For $1 \leq j \leq k-1$, the multiplicity of each eigenvalue of $T_j$ as an eigenvalue of $A_\alpha(C_r\{B(d,k)\})$ is $rd^{k-j-1}(d-1)$, and for $1 \leq i \leq r$, the eigenvalues of $S_i$ as eigenvalues of $A_\alpha(C_r\{B(d,k)\})$ are simple. If some eigenvalues obtained in different matrices are equal, their multiplicities are added together.

3. The largest eigenvalue of
   \[
   S_i = \begin{bmatrix}
   \alpha & \beta\sqrt{d} & 0 & 0 \\
   \beta\sqrt{d} & \alpha(d+1) & \beta\sqrt{d} & \cdot \\
   \cdot & \cdot & \cdot & \cdot \\
   0 & 0 & \beta\sqrt{d} & \alpha(d+1)
   \end{bmatrix}
   \]
   is the spectral radius of $A_\alpha(C_r\{B(d,k)\})$.

Let $\rho(M)$ be the spectral radius of the matrix $M$. It is known that if $G$ is a subgraph of $H$ then $\rho(L(G)) \leq \rho(L(H))$, $\rho(Q(G)) \leq \rho(Q(H))$ and $\rho(A(G)) \leq \rho(A(H))$.

In [10] Stevanović proves that for a tree $T$ with largest vertex degree $\Delta$,

\[
\rho(L(T)) < \Delta + 2\sqrt{\Delta - 1}
\]

and

\[
\rho(A(T)) < 2\sqrt{\Delta - 1}.
\]

In [5] Hu proves that if $G$ is a unicyclic graph with largest vertex degree $\Delta$ then

\[
\rho(L(G)) \leq \Delta + 2\sqrt{\Delta - 1}
\]

with equality if and only if $G$ is the cycle $C_n$ whenever $n$ is even, and

\[
\rho(A(G)) \leq 2\sqrt{\Delta - 1}
\]

with equality if and only if $G$ is the cycle $C_n$.

From now on, let $G = (V(G), E(G))$ be a unicyclic graph with largest vertex degree $\Delta$.

We recall that the height of a rooted tree is the largest distance from its root to a pendant vertex. The following invariant for a unicyclic graph $G$ was introduced in [9].

**Definition 14** Let $G$ be a unicyclic graph. Let $C_r$ be the unique cycle in $G$ and let $v_1, v_2, \ldots, v_r$ be the vertices of $C_r$. The graph $G - E(G)$ is a forest of $r$ rooted trees $T_1, T_2, \ldots, T_r$ with roots $v_1, \ldots, v_r$, respectively. For $i = 1, 2, \ldots, r$, let $h(T_i)$ be the height of the tree $T_i$. Let

\[
k(G) = \max \{ h(T_i) : 1 \leq i \leq r \} + 1.
\]

We say that $k(G)$ is the height of the unicyclic $G$. 9
**Example 15** Let $G$ be the unicyclic graph:

![Graph Image]

Then $\Delta(G) = 5$ and the height of $G$ is

$$k(G) = \max\{3, 2, 1, 4, 2\} + 1 = 5,$$

In [9] the upper bounds given in (8) and (9) are improved as follows:

**Lemma 16** If $G$ is a unicyclic graph then

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

(10)

for $\Delta \geq 3$ and

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

(11)

for $\Delta \geq 4$ or $\Delta = 3$ and $k(G) \geq 4$.

It is well known [2] that

$$\rho(L(G)) \leq \rho(Q(G))$$

with equality if and only if $G$ is a bipartite graph. In [3] upper bounds on $\rho(L(G))$ and $\rho(Q(G))$ are given and it is proved that many but not all upper bounds on $\rho(L(G))$ are also bounds for $\rho(Q(G))$. In [1] it is shown that if $G$ is a unicyclic graph, the upper bound on $\rho(L(G))$ in (10) is also an upper bound on $\rho(Q(G))$.

**Lemma 17** Let $\Delta \geq 3$. Let

$$X = \begin{bmatrix}
0 & \sqrt{\Delta - 1} & & \\
\sqrt{\Delta - 1} & 0 & \ddots & \\
& \ddots & \ddots & \sqrt{\Delta - 1} \\
& & \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 2} \\
& & & \sqrt{\Delta - 2} & 2
\end{bmatrix}$$

be a tridiagonal matrix of order $k \times k$. If $\Delta \geq 4$ or $\Delta = 3$ with $k \geq 4$ then

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

(12)
Proof Let
\[
Y = \begin{bmatrix}
0 & \sqrt{\Delta - 1} & & \\
\sqrt{\Delta - 1} & 0 & \ddots & \\
& \ddots & \ddots & \sqrt{\Delta - 1} \\
& & \sqrt{\Delta - 1} & 0 & \sqrt{\Delta - 1} \\
& & & \sqrt{\Delta - 1} & \\
\end{bmatrix}
\]
be a symmetric tridiagonal matrix of order \(k \times k\). It is known [6] that
\[
\rho(Y) = 2\sqrt{\Delta - 1} \cos \frac{\pi}{2k+1}.
\]
Hence proving (12) is equivalent to proving that \(\rho(X) < \rho(Y)\). Suppose that \(\Delta \geq 5\). Then \(X \leq Y\) with strict inequalities in the entries \((k-1,k)\) and \((k,k-1)\). Since the spectral radius of an irreducible nonnegative matrix increases when any of its entries increases, we have \(\rho(X) < \rho(Y)\). Thus, (12) has been proved for \(\Delta \geq 5\). For \(j = 1, 2, \ldots, k\), let \(x_j(\lambda)\) and \(y_j(\lambda)\) be the characteristic polynomials of the \(j \times j\) leading principal submatrices of \(X\) and \(Y\), respectively. Notice that \(x_j(\lambda)\) and \(y_j(\lambda)\) are identical polynomials for \(j = 1, 2, \ldots, k-1\). Using the three-term recursion formula for symmetric tridiagonal matrices, we have
\[
x_k(\lambda) = (\lambda - 2)x_{k-1}(\lambda) - (\Delta - 2)x_{k-2}(\lambda)
\]
and
\[
y_k(\lambda) = (\lambda - \sqrt{\Delta - 1})x_{k-1}(\lambda) - (\Delta - 1)x_{k-2}(\lambda).
\]
Subtracting (14) from (13), we obtain
\[
x_k(\lambda) - y_k(\lambda) = (\sqrt{\Delta - 1} - 2)x_{k-1}(\lambda) + x_{k-2}(\lambda).
\]
Since \(X\) and \(Y\) are symmetric tridiagonal matrices with nonzero codiagonal entries, their eigenvalues are simple. Let
\[
a_k < a_{k-1} < \ldots < a_2 < \rho(X)
\]
be the eigenvalues of \(X\). Then
\[
x_k(\lambda) = (\lambda - \rho(X)) \prod_{j=2}^{k} (\lambda - a_j).
\]
Let \(\beta_1\) be the largest zero of the identical polynomials \(x_{k-1}(\lambda)\) and \(y_{k-1}(\lambda)\). Since the zeros of these polynomials strictly interlace the zeros of the polynomials \(x_k(\lambda)\) and \(y_k(\lambda)\), we have \(a_2 < \beta_1 < \rho(X)\) and \(\beta_1 < \rho(Y)\). Therefore \(a_2 < \rho(Y)\), \(x_{k-1}(\rho(Y)) > 0\) and
\[
x_k(\rho(Y)) = (\rho(Y) - \rho(X))c,
\]
where \[ c = \prod_{j=2}^{k} (\rho(Y) - a_j) > 0. \]

Thus in order to conclude that \( \rho(X) < \rho(Y) \), we need to show that \( x_k(\rho(Y)) > 0 \). From (14) and (15),

\[ y_k(\rho(Y)) = 0 = (\rho(Y) - \sqrt{\Delta - 1})x_{k-1}(\rho(Y)) - (\Delta - 1)x_{k-2}(\rho(Y)) \]

and

\[ x_k(\rho(Y)) = (\sqrt{\Delta - 1} - 2)x_{k-1}(\rho(Y)) + x_{k-2}(\rho(Y)). \]

Then

\[ x_k(\rho(Y)) = (\sqrt{\Delta - 1} - 2 + \frac{\rho(Y) - \sqrt{\Delta - 1}}{\Delta - 1})x_{k-1}(\rho(Y)). \tag{16} \]

Let \( \Delta = 4 \). From (16)

\[ x_k(\rho(Y)) = (\sqrt{3} - 2 + 2\sqrt{3}\cos\frac{\pi}{2k+1} - \sqrt{3})x_{k-1}(\rho(Y)) \]

\[ = (\frac{2\sqrt{3}}{3} - 2 + 2\sqrt{3}\cos\frac{\pi}{2k+1})x_{k-1}(\rho(Y)) \]

\[ \geq (\frac{2\sqrt{3}}{3} - 2 + 2\sqrt{3}\cos\frac{\pi}{5})x_{k-1}(\rho(Y)) > 0.08x_{k-1}(\rho(Y)) > 0. \]

It remains to prove (12) for \( \Delta = 3 \) and \( k \geq 4 \). From (16)

\[ x_k(\rho(Y)) = (\sqrt{2} - 2 + 2\sqrt{2}\cos\frac{\pi}{2k+1} - \sqrt{2})x_{k-1}(\rho(Y)) \]

\[ = (\frac{\sqrt{2}}{2} - 2 + \sqrt{2}\cos\frac{\pi}{2k+1})x_{k-1}(\rho(Y)) \]

\[ \geq (\frac{\sqrt{2}}{2} - 2 + \sqrt{2}\cos\frac{\pi}{9})x_{k-1}(\rho(Y)) > 0.03x_{k-1}(\rho(Y)) > 0. \]

The proof of Lemma 17 is complete.

At this point, we observe that if \( G \) is an induced subgraph of \( H \) then \( A_{\alpha}(G) \leq A_{\alpha}(H) \).

The next theorem gives an upper bound on the spectral radius of \( A_{\alpha}(G) \) in terms of the largest degree and height of the unicyclic graph \( G \).

**Theorem 18** Let \( G \) be a unicyclic graph with \( \Delta \geq 3 \). Let \( \alpha \in [0, 1] \). If \( \Delta \geq 4 \) or \( \Delta = 3 \) and \( k(G) \geq 4 \) then

\[ \rho(A_{\alpha}(G)) < \alpha\Delta + 2(1 - \alpha)\sqrt{\Delta - 1}\cos\frac{\pi}{2k(G) + 1} \tag{17} \]

**Proof** Let \( C_r \) be the unique cycle in \( G \). Let \( H = B_{k(G)} \) be a generalized Bethe tree with vertex degrees

\[ d_1 = 1, d_2 = \Delta, \ldots, d_{k(G)-1} = \Delta, d_{k(G)} = \Delta - 2 \]

\[ \square \]
from the pendant vertices to the root. Then $G$ is an induced subgraph of $C_r\{H\}$. Hence $\rho(A_\alpha(G)) \leq \rho(A_\alpha(C_r\{H\}))$. Let $\beta = 1 - \alpha$. From Corollary 12, the spectral radius of $A_\alpha(C_r\{H\})$ is the spectral radius of the $k(G) \times k(G)$ matrix

$$S_1 = \begin{bmatrix}
\alpha & \beta \sqrt{\Delta - 1} \\
\beta \sqrt{\Delta - 1} & \alpha \Delta \\
\beta \sqrt{\Delta - 1} & \alpha \Delta & \ddots \\
\ddots & \ddots & \ddots & \beta \sqrt{\Delta - 1} \\
\beta \sqrt{\Delta - 1} & \alpha \Delta & \beta \sqrt{\Delta - 1} & \beta \sqrt{\Delta - 1} & \alpha \Delta + 2 \beta
\end{bmatrix}.$$  

We have

$$S_1 \leq \begin{bmatrix}
\alpha \Delta & \beta \sqrt{\Delta - 1} \\
\beta \sqrt{\Delta - 1} & \alpha \Delta \\
\beta \sqrt{\Delta - 1} & \alpha \Delta & \ddots \\
\ddots & \ddots & \ddots & \beta \sqrt{\Delta - 1} \\
\beta \sqrt{\Delta - 1} & \alpha \Delta & \beta \sqrt{\Delta - 1} & \beta \sqrt{\Delta - 1} & \alpha \Delta + 2 \beta
\end{bmatrix} + \alpha \begin{bmatrix}
\Delta \\
\Delta \\
\ddots \\
\ddots \\
\Delta
\end{bmatrix} + \beta \begin{bmatrix}
0 & \sqrt{\Delta - 1} \\
\sqrt{\Delta - 1} & \ddots \\
\ddots & \ddots & \sqrt{\Delta - 1} \\
\sqrt{\Delta - 2} & \ddots & \ddots & \ddots \\
\sqrt{\Delta - 2} & 2
\end{bmatrix} + \beta \begin{bmatrix}
\Delta \\
\Delta \\
\ddots \\
\ddots \\
\Delta
\end{bmatrix}$$

where $X$ is as in Lemma 17. Then

$$\rho(S_1) \leq \alpha \Delta + \beta \rho(X).$$
If $\Delta \geq 4$ and $\Delta = 3$ with $k(G) \geq 4$, applying Lemma 17, the upper bound (17) follows.

Finally we study the cases $\Delta = 3$ and $k(G) \leq 3$. In [9] it is observed that the upper bound (17) does not hold for the adjacency matrix ($\alpha = 0$) when $\Delta = 3$ if $k(G) = 3$ or $k(G) = 2$.

Let $\alpha \neq 0$ and $\Delta = 3$. Let $k(G) = 3$ or $k(G) = 2$. From Corollary 12, the spectral radius of $A_{\alpha}(C_r\{H\})$ is the spectral radius of the $3 \times 3$ matrix

$$M_3 = S_1 = \begin{bmatrix} \alpha & \beta \sqrt{2} & 0 \\ \beta \sqrt{2} & 3\alpha & \beta \\ 0 & \beta & \alpha + 2 \end{bmatrix}.$$ 

or of the $2 \times 2$ matrix

$$M_2 = S_1 = \begin{bmatrix} \alpha & \beta \\ \beta & \alpha + 2 \end{bmatrix}.$$ 

We have

$$M_3 = \begin{bmatrix} \alpha & \beta \sqrt{2} & 0 \\ \beta \sqrt{2} & 3\alpha & \beta \\ 0 & \beta & \alpha + 2 \end{bmatrix} = \begin{bmatrix} 3\alpha & 0 & 0 \\ 0 & 3\alpha & 0 \\ 0 & 0 & 3\alpha \end{bmatrix} + \begin{bmatrix} -2\alpha & \beta \sqrt{2} & 0 \\ \beta \sqrt{2} & 0 & \beta \\ 0 & \beta & 2\beta \end{bmatrix}.$$ 

Then

$$\rho(M_3) = 3\alpha + \beta \rho(Z(\gamma))$$

where

$$Z(\gamma) = \begin{bmatrix} \gamma & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

with $\gamma = -2\frac{\alpha}{\beta}$. Similarly

$$M_2 = \begin{bmatrix} \alpha & \beta \\ \beta & \alpha + 2 \end{bmatrix} = \begin{bmatrix} 3\alpha & 0 \\ 0 & 3\alpha \end{bmatrix} + \begin{bmatrix} \delta & 1 \\ 1 & 2 \end{bmatrix}$$

where $\delta = -2\frac{\alpha}{\beta}$. Then

$$\rho(M_2) = 3\alpha + \beta \rho(W(\delta))$$

where

$$W(\delta) = \begin{bmatrix} \delta & 1 \\ 1 & 2 \end{bmatrix}.$$ 

We recall a simplified version of the Weyl’s inequalities for eigenvalues of Hermitian matrices (see, e.g. [4], p. 181).
**Lemma 19** Let $A$ and $B$ be Hermitian matrices of order $n \times n$. Let $C = A + B$. Let

$$\alpha_1 \geq \alpha_2 \geq \ldots \alpha_n,$$

$$\beta_1 \geq \beta_2 \geq \ldots \beta_n$$

and

$$\gamma_1 \geq \gamma_2 \geq \ldots \gamma_n$$

be the eigenvalues of $A$, $B$ and $C$, respectively. Then, for $j = 1, 2, \ldots, n$,

$$\alpha_j + \beta_n \leq \gamma_j \leq \alpha_j + \beta_1. \quad (18)$$

In either of these inequalities equality holds if and only if there exists a nonzero $n$-vector that is an eigenvector to each of the three eigenvalues involved. The conditions for equality in Weyl’s inequalities were first established by So in [11].

We have

$$Z(x) = \begin{bmatrix} x - y & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + Z(y).$$

We claim that $\rho(Z(\gamma))$ is a strictly increasing function of $\gamma$. In fact, for $x < y$, Weyl’s inequalities imply that

$$\rho(Z(x)) < 0 + \rho(Z(y)) = \rho(Z(y)).$$

A similar argument shows that $\rho(W(\delta))$ is a strictly increasing function of $\delta$. Numerical computations show that $\rho(Z(-0.25)) < 2\sqrt{2} \cos \frac{\pi}{7}$ and $\rho(Z(-0.2)) > 2\sqrt{2} \cos \frac{\pi}{7}$; and, $\rho(W(-1.2)) < 2\sqrt{2} \cos \frac{\pi}{5}$ and $\rho(W(-1.1)) > 2\sqrt{2} \cos \frac{\pi}{5}$. Since $\rho(Z(\gamma))$ and $\rho(W(\delta))$ are continuous functions, there exists $\gamma_0 \in (-0.25, -0.2)$ such that $\rho(Z(\gamma_0)) = 2\sqrt{2} \cos \frac{\pi}{7}$ and there exists $\delta_0 \in (-1.2, -1.1)$ such that $\rho(W(\delta_0)) = 2\sqrt{2} \cos \frac{\pi}{5}$.

**Theorem 20** Let $G$ be a unicyclic graph. Let $\Delta = 3$. If $\alpha > -\frac{\gamma_0}{2-\gamma_0}$ whenever $k(G) = 3$ or if $\alpha > -\frac{\delta_0}{2-\delta_0}$ whenever $k(G) = 2$, then the upper bound (17) holds.

**Proof** Let $k(G) = 3$. There exists $\gamma_0$ such that $\rho(Z(\gamma_0)) = 2\sqrt{2} \cos \frac{\pi}{7}$. Moreover, $\rho(Z(\gamma))$ is a strictly increasing function. Hence

$$\rho(Z(\gamma)) < 2\sqrt{2} \cos \frac{\pi}{7}$$

for $\gamma < \gamma_0$. We recall that $\gamma = -\frac{2\alpha}{1-\alpha}$. Imposing the inequality

$$-\frac{2\alpha}{1-\alpha} < \gamma_0$$

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we obtain $\alpha > \frac{\gamma_0}{\gamma_0^2 - \gamma_0}$. Hence for such values of $\alpha$, we have

$$\rho(A_\alpha(C_r\{H\})) = \rho(M_3) = 3\alpha + \beta\rho(Z(\gamma)) < 3\alpha + 2(1 - \alpha)\sqrt{2}\cos\frac{\pi}{7}.$$ 

Then the upper bound (17) holds whenever $k(G) = 3$ and $\Delta = 3$. The proof for the case $k(G) = 2$ is similar.

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