On the Randić energy of caterpillar graphs

Domingos M. Cardoso, Paula Carvalho, Roberto C. Díaz, Paula Rama

Abstract

A caterpillar graph $T(p_1, \ldots, p_r)$ of order $n = r + \sum_{i=1}^{r} p_i$, $r \geq 2$, is a tree such that removing all its pendent vertices gives rise to a path of order $r$. In this paper we establish a necessary and sufficient condition for a real number to be an eigenvalue of the Randić matrix of $T(p_1, \ldots, p_r)$. This result is applied to determine the extremal caterpillars for the Randić energy of $T(p_1, \ldots, p_r)$ for cases $r = 2$ (the double star) and $r = 3$. We characterize the extremal caterpillars for $r = 2$. Moreover, we study the family of caterpillars $T(p, n-p-3, q)$ of order $n$, where $q$ is a function of $p$, and we characterize the extremal caterpillars for three cases: $q = p$, $q = n - p - 3$ and $q = b$, for $b \in \{1, \ldots, n-6\}$ fixed. Some illustrative examples are included.

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1 Introduction

It is worth to start this section defining the Randić matrix of a graph $G$, denoted by $R_G = (r_{ij})$, which is such that $r_{ij} = \frac{1}{\sqrt{d_id_j}}$ if $ij \in E(G)$ and zero otherwise, where $d_k$ is the degree of the vertex $k$. The spectrum of $R_G$ is the multiset of its eigenvalues, $\sigma_{R}(G) = \{\rho_1^{[m_1]}, \rho_2^{[m_2]}, \ldots, \rho_s^{[m_s]}\}$, where $m_i$ stands for the multiplicity of $\rho_i$, for $1 \leq i \leq s$, and $\rho_1 > \rho_2 > \cdots > \rho_s$ are the distinct eigenvalues of $R_G$.

It is well known that $\rho_1(G) = 1$ whenever $G$ is a graph with at least one edge (see [7, Th. 2.3]). The Randić energy of a graph $G$ is defined in [7] (see also [2, 3]) as follows:

$$RE(G) = \sum_{i=1}^{n} |\rho_i(G)|.$$
It is immediate that $RE(G) = 0$ if and only if all the vertices of $G$ are isolated vertices. Considering $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ as the eigenvalues of the adjacency matrix of a graph $G$ of order $n$, the ordinary energy of $G$ [8,11], herein denoted by $\mathcal{E}(G)$, is defined as

$$\mathcal{E}(G) = \sum_{j=1}^{n} |\lambda_j|.$$  

In [7], the Randić energy and the ordinary energy of the paths $P_n$ and $P_{n-2}$, respectively, are related as follows.

$$RE(P_n) = 2 + \frac{1}{2} \mathcal{E}(P_{n-2}).$$

According to [5], if a graph $G$ of order $n$ has at least one edge, then

$$2 \leq RE(G) \leq n. \quad (1.1)$$

Furthermore, the lower bound in (1.1) is attained if and only if one component of $G$ is a complete multipartite graph and all other components (if any) are isolated vertices. In particular, $RE(G) = 2$ for complete graphs. The upper bound in (1.1) is attained only if $n$ is even and $G$ is isomorphic to $\frac{n}{2}K_2$, or $n$ is odd and $G$ is the disjoin union of $\frac{n-3}{2}K_2$ and a component which is a path $P_2$ or a triangle $K_3$.

The characterization of connected graphs with maximal Randić energy remains an open problem as well as the following conjecture posed in [7] and computationally verified for graphs of order $n$ up to $n = 10$.

**Conjecture 1** [7] *The connected graph with maximal Randić energy is a tree.*

The following more thinner conjecture, also posed in [7], remains open too.

**Conjecture 2** [7] *The connected graph of odd order $n \geq 1$, having maximal Randić energy is the sun [7, Fig. 2]. The connected graph of even order $n \geq 2$, having maximal Randić energy is the balanced double sun [7, Fig. 2].*

The aim of this paper is to determine the extremal graphs for the Randić energy of a family of caterpillars $T(p_1, \ldots, p_r)$ of order $n = r + \sum_{i=1}^{r} p_i$ for cases $r = 2$ and $r = 3$. The paper is organized as follows. In Section 2 the notation and basic definitions of the main concepts used through the text are introduced. In Section 3 a caterpillar is consider as the H-join of graphs and some spectral results of graphs obtained by this operation are recalled. Moreover, we get a necessary and sufficient condition for a real number to be an eigenvalue of the Randić matrix. This result plays an important role throughout the paper. In Section 4 we characterize the extremal caterpillar graphs for $r = 2$ (that are the double star) as well as we study the family of caterpillars $T(p, n - p - q - 3, q)$ of order $n$, and we characterize extremal caterpillar graphs for three cases: $q = p$, $q = n - p - b - 3$ and $q = b$, for any $b \in \{1, \ldots, n - 6\}$ fixed.
2 Preliminaries

In this paper we deal with undirected simple graphs. For a graph $G$ the vertex set is denoted by $V(G)$ and the edge set by $E(G)$ and $|V(G)|$ is the order of $G$. The edges of $G$ denoted by $ij$, where $i$ and $j$ are the end-vertices of the edge. When $ij \in E(G)$ we say that the vertices $i$ and $j$ are adjacent and also that $i$ is a neighbor of $j$ (and conversely). The neighborhood of a vertex $v \in V(G)$ is the set of its neighbors and is denoted by $N_G(v) = \{ w : vw \in E(G) \}$. The degree of $v$, denoted by $d_v$, is the cardinality of $N_G(v)$. The vertices $i$ with 0 degree are called isolated vertices. Two graphs $G$ and $H$ are isomorphic if there is a bijection $\psi : V(G) \rightarrow V(H)$ such that $ij \in E(G)$ if and only if $\psi(i)\psi(j) \in E(H)$. This binary relation between graphs is denoted by $G \cong H$. The complement graph of a graph $G$, denoted by $\overline{G}$, is such that $V(\overline{G}) = V(G)$ and $E(\overline{G}) = \{ ij : ij \notin E(G) \}$. The complete graph of order $n$, denote by $K_n$, is a graph where every pair of vertices are adjacent. The vertices of the complement of $K_n$ are all isolated. The adjacency matrix of a graph $G$ of order $n = |V(G)|$ is $n \times n$ symmetric matrix $A_G = (a_{ij})$ such that $a_{ij} = 1$ if $ij \in E(G)$ and zero otherwise. The spectrum of a matrix $M$ is the multiset of its eigenvalues denoted by $\sigma_M$. In particular, the spectrum of the adjacency matrix of a graph $G$, also called the spectrum of $G$, is $\sigma(G) = \{ \lambda_1^{[m_1]}, \lambda_2^{[m_2]}, \ldots, \lambda_s^{[m_s]} \}$, where $m_i$ stands for the multiplicity of $\lambda_i$, for $1 \leq i \leq s$.

A path with $r$ vertices, denoted by $P_r$, is a sequence of vertices $v_1, v_2, \ldots, v_r$ such that each vertex is adjacent to the next, that is, $v_iv_{i+1} \in E(G)$ for $i = 1, \ldots, r - 1$. A cycle $C_r$ is a closed path with $r$ edges, that is, such that $v_{r+1} = v_1$. A tree is a connected acyclic graph; a star of order $r$, denoted by $S_r$, is a tree with a central vertex with degree $r$ and all the other $r$ vertices are pendant. A caterpillar is a tree such that removing all pendant vertices give rise to a path with at least two vertices. In particular, $T(p_1, \ldots, p_r)$ denotes a caterpillar obtained by attaching the central vertex of a star $S_{p_i+1}$ to the $i$-th vertex of $P_r$, $i = 1, \ldots r$. The order of a caterpillar is $n = r + \sum_{i=1}^r p_i$.

A caterpillar $T(p_1, \ldots, p_r)$ can also be seen as the $H$-join $H[G_1, \ldots, G_r, G_{r+1}, \ldots, G_{2r}]$, where, for $1 \leq i \leq r$, \begin{equation*}
G_i \cong \begin{cases} K_1 & \text{and } H \text{ is the caterpillar of order } 2r, \ T(1, \ldots, 1), \text{that is, a path } P_r \\
G_{i+r} \cong K_{p_i} & \text{with one pendant vertex attached to each vertex of the path.}
\end{cases}
\end{equation*}

The null square and the identity matrices of order $n$ are denoted by $O_n$ and $I_n$, respectively.

3 The Randić spectrum of a caterpillar viewed as $H$-join

In this section, we consider a caterpillar as the $H$-join of a family of graphs (see [4]), $T(p_1, \ldots, p_r) = H[K_1, \ldots, K_1, \overline{K_{p_1}}, \ldots, \overline{K_{p_r}}]$, where $H$ is the caterpillar of order $2r$, $T(1, 1, \ldots, 1)$, that is, a path $P_r$ with a pendant edge attached to each vertex of the path. The following result, given in [1], characterizes Randić spectra of $H$-join graphs.

**Theorem 3.1** [1] Let $H$ be a graph of order $k$. Let $G_j$ be a $d_j$-regular graph of order $n_j$, with
Corollary 3.1 plays an important role in this paper:

$$H\Omega = \text{diag} \{\lambda \in \sigma(A_{G_j}) \setminus \{d_j\}\},$$

where $N_j = \sum_{i\in N_H(j)} n_i$, for $j = 1, 2, \ldots, k$,

$$\Gamma_k = \begin{pmatrix}
\frac{d_1}{N_1+d_1} & \rho_{12} & \cdots & \rho_{1(k-1)} & \rho_{1k} \\
\rho_{12} & \frac{d_2}{N_2+d_2} & \cdots & \rho_{2(k-1)} & \rho_{2k} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
\rho_{1(k-1)} & \rho_{2(k-1)} & \cdots & \frac{d_{k-1}}{N_{k-1}+d_{k-1}} & \rho_{(k-1)k} \\
\rho_{1k} & \rho_{2k} & \cdots & \rho_{(k-1)k} & \frac{d_k}{N_k+d_k}
\end{pmatrix}$$

and

$$\rho_{ij} = \delta_{ij} \sqrt{\frac{n_in_j}{(N_i+d_i)(N_j+d_j)}},$$

with $\delta_{ij} = 1$ if $ij \in E(H)$, and zero otherwise, for $i = 1 \ldots, k-1$ and $j = i + 1, \ldots, k$.

Remark 1 It is clear that the Randić matrix of a $d_j$-regular graph $G_j$ is $R_{G_j} = \frac{1}{d_j}A_{G_j}$ if $d_j > 0$ and zero otherwise. On the other hand, if $d_j = 0$, for $j = 1, \ldots, k$, then $\Gamma_k = \Omega A_{H}\Omega$, with $\Omega = \text{diag}\{\sqrt{\frac{n_1}{N_1}}, \ldots, \sqrt{\frac{n_k}{N_k}}\}$.

Since $K_1$ and $K_{p_i}$, for $i = 1, \ldots, r$, are 0-regular graphs, we have the following result, which plays an important role in this paper:

Corollary 3.1 Let $H = T(1,1,\ldots,1)$ be the caterpillar of order $2r$, $r \geq 2$, obtained from a path $P_r$ and a pendent vertex attached to each vertex of the path. Let $T = T(p_1,\ldots,p_r) = H[K_1,\ldots,K_1,K_{p_1},\ldots,K_{p_r}]$ be a caterpillar of order $n = r + \sum_{i=1}^{r} p_i$. Then,

$$\sigma_{R_T} = \sigma_{\Gamma_{2r}} \cup \{0|\sum_{i=1}^{r} (p_i-1)|\}.$$ 

As a consequence, in order to obtain the spectrum of the Randić matrix of $T(p_1,\ldots,p_r)$ we focus our attention on the spectrum of $\Gamma_{2r}$. Firstly, note that

$$\Omega = \text{diag}\left\{\sqrt{\frac{1}{N_1}}, \ldots, \sqrt{\frac{1}{N_r}}, \sqrt{\frac{p_1}{N_{r+1}}}, \ldots, \sqrt{\frac{p_r}{N_{2r}}}\right\} = \begin{bmatrix} \Omega_1 & O_r \\ O_r & \Omega_2 \end{bmatrix}$$

with

$$\Omega_1 = \text{diag}\left\{\sqrt{\frac{1}{N_1}}, \ldots, \sqrt{\frac{1}{N_r}}\right\}, \quad \Omega_2 = \text{diag}\left\{\sqrt{\frac{p_1}{N_{r+1}}}, \ldots, \sqrt{\frac{p_r}{N_{2r}}}\right\}, \quad (3.1)$$

Therefore, we can write

$$\Gamma_{2r} = \Omega A_H \Omega = \begin{bmatrix} \Omega_1 & O_r \\ O_r & \Omega_2 \end{bmatrix} \begin{bmatrix} A_{P_r} & I_r \\ I_r & O_{r+j} \end{bmatrix} \begin{bmatrix} \Omega_1 & O_r \\ O_r & \Omega_2 \end{bmatrix} = \begin{bmatrix} A & B \\ B & O_r \end{bmatrix}, \quad (3.2)$$
where

\[ A = \Omega_1 A_{p_r}, \Omega_1 \quad \text{and} \quad B = \Omega_1 \Omega_2. \] (3.3)

It is worth to recall a famous determinantal identity presented by Issa Schur in 1917 [12] referred as the formula of Schur by Gantmacher [6, p. 46]. In the sixties, the term Schur complement was introduced by Emilie Haynsworth [9] jointly with the following notation. Considering a square matrix \( M = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \), where \( A \) and \( D \) are square block matrices and \( A \) is nonsingular, the Schur complement of \( A \) in \( M \) is defined as

\[ M/A = D - CA^{-1}B. \]

For more details see [10]. Using the above notation, the next theorem states the Schur determinantal identity. For the readers convenience, the very short proof presented in [10] is reproduced.

**Theorem 3.2** [12] Let \( M = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \), where \( A \) and \( D \) are square submatrices of order \( m \) and \( n \), respectively. If \( A \) is nonsingular then

\[ \det(M) = \det(A) \cdot \det(M/A). \]

**Proof** It is immediate that

\[ \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I_m & 0 \\ CA^{-1} & I_n \end{bmatrix} \begin{bmatrix} A & B \\ 0 & D - CA^{-1}B \end{bmatrix}. \]

The identity follows by taking the determinant of both sides. \( \square \)

Similarly, if \( D \) is nonsingular then

\[ \det(M) = \det(A - BD^{-1}C) \cdot \det(D). \] (3.4)

Note that

\[ \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I_m & BD^{-1} \\ 0 & I_n \end{bmatrix} \begin{bmatrix} A - BD^{-1}C & 0 \\ C & D \end{bmatrix}. \]

From (3.4), we may establish the following spectral characterization for the matrix \( \Gamma_{2r} \), which will play an important role in getting our main results:

**Theorem 3.3** Let \( H = T(1, 1, \ldots, 1) \) be the caterpillar of order \( 2r \), \( r \geq 2 \) and let \( \Gamma_{2r} \) be partitioned as in (3.2). Then, \( \lambda \in \sigma_{\Gamma_{2r}} \) if and only if

\[ \det(\lambda^2 I_r - \lambda A - B^2) = 0, \]

where \( A \) and \( B \) are defined as in (3.3).
Proof The characteristic polynomial of $\Gamma_{2r}$ is

$$p_{\Gamma_{2r}}(\lambda) = \det(\lambda I_{2r} - \Gamma_{2r}) = \det \left( \begin{bmatrix} \lambda I_r - A & -B \\ -B & \lambda I_r \end{bmatrix} \right).$$

Thus, applying (3.4), we obtain

$$p_{\Gamma_{2r}}(\lambda) = \det(\lambda I_r) \cdot \det \left( \lambda I_r - A - B \left( \frac{1}{\lambda} I_r \right) B \right)$$

$$= \lambda^r \cdot \det \left( \frac{1}{\lambda} \right) (\lambda^2 I_r - \lambda A - B^2)$$

$$= \lambda^r \left( \frac{1}{\lambda} \right)^r \cdot \det (\lambda^2 I_r - \lambda A - B^2) = \det (\lambda^2 I_r - \lambda A - B^2).$$

\[\square\]

4 Extremal caterpillar graphs for Randić energy

In this section, we obtain the extremal graphs in the family of caterpillars, for $r = 2, 3$.

4.1 Extremal caterpillar graphs $T(p, n - p - 2)$, $p = 1, \ldots, \left\lfloor \frac{n-2}{2} \right\rfloor$.

Theorem 4.1 Let $T_p = T(p, n - p - 2)$, $p = 1, \ldots, \left\lfloor \frac{n-2}{2} \right\rfloor$ be a caterpillar of order $n \geq 4$. Then

$$2 + \sqrt{\frac{2(n-3)}{n-2}} \leq RE(T_p) \leq 4 - \frac{4}{n}.$$

The lower bound is attained if and only if $p = 1$ (the graph obtained by attaching a pendent vertex to a pendent vertex of $S_{n-1}$) and the upper bound is attained if and only if $T_p$ has even order and $p = \frac{n-2}{2}$.

Proof By Theorem 3.3, the eigenvalues of $\sigma_4$ are the zeros of the polynomial $\det(\lambda^2 I_2 - \lambda A - B^2) = 0$ where (see (3.3)),

$$A = \begin{bmatrix} 0 & \frac{1}{\sqrt{(p+1)(n-p-1)}} \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} \frac{\sqrt{p}}{\sqrt{p+1}} & 0 \\ 0 & \frac{\sqrt{n-p-2}}{\sqrt{n-p-1}} \end{bmatrix}. $$

6
So,
\[
\det(\lambda^2 I_2 - \lambda A - B^2) = \det \begin{bmatrix}
-\lambda^2 - \frac{p}{p+1} & -\sqrt{\frac{(p+1)(n-p-1)}{\lambda^2 - \frac{n-p-2}{n-p-1}}} \\
\sqrt{\frac{(p+1)(n-p-1)}{\lambda^2 - \frac{n-p-2}{n-p-1}}} & -\lambda
\end{bmatrix}
\]
\[
= \left(\lambda^2 - \frac{p}{p+1}\right) \left(\lambda^2 - \frac{n-p-2}{n-p-1}\right) - \frac{\lambda^2}{(p+1)(n-p-1)} \left[(p+1)(n-p-1)\lambda^2 - p(n-p-2)\right].
\]
Consequently,
\[
\sigma_{\Gamma_4} = \left\{ \pm \sqrt{\frac{p(n-p-2)}{(p+1)(n-p-1)}}, \pm 1 \right\}.
\]
and
\[
RE(T_p) = \sum_{i=1}^{n} |\lambda_i(T_p)| = 2 + 2\sqrt{\frac{p(n-p-2)}{(p+1)(n-p-1)}},
\]
for all \(p = 1, \ldots, \left\lfloor \frac{n-2}{2} \right\rfloor\). For \(1 \leq x \leq \left\lfloor \frac{n-2}{2} \right\rfloor\), let \(f(x) = \frac{x(n-x-2)}{(x+1)(n-x-1)}\). Then,
\[
f'(x) = \frac{(n-1)(n-2(x+1))}{(x+1)^2(n-x-1)^2} \geq 0.
\]
if and only if \(1 \leq x \leq \frac{n-2}{2}\). Therefore, \(f\) is an increasing function in this interval, and consequently,
\[
2 + \sqrt{\frac{2(n-3)}{n-2}} \leq RE(T_p) \leq RE(T_{\left\lfloor \frac{n-2}{2} \right\rfloor}),
\]
for all \(p = 1, \ldots, \left\lfloor \frac{n-2}{2} \right\rfloor\). Finally, if \(n\) is even,
\[
RE(T_{\left\lfloor \frac{n-2}{2} \right\rfloor}) = RE(T_{\frac{n-2}{2}}) = 2 + 2\left(\frac{n-2}{n}\right) = 4 - \frac{4}{n},
\]
and if \(n\) is odd,
\[
RE(T_{\left\lfloor \frac{n-2}{2} \right\rfloor}) = RE(T_{\left\lfloor \frac{n-3}{2} + \frac{1}{2} \right\rfloor}) = RE(T_{\frac{n-3}{2}}) = 2 + 2\left(\frac{n-3}{n+2}\right) < 4 - \frac{4}{n}
\]
for all \(n \geq 3\).

\[\square\]

4.2 Extremal caterpillar graphs \(T(p, n - p - q - 3, q)\), \(p, q \in \{1, \ldots, n - 5\}\)
For this class of caterpillars,

\[ \Omega_1 = \text{diag} \left\{ \frac{1}{\sqrt{p+1}}, \frac{1}{\sqrt{n-p-q-1}}, \frac{1}{\sqrt{q+1}} \right\} \]

and

\[ \Omega_2 = \text{diag} \left\{ \sqrt{p}, \sqrt{n-p-q-3}, \sqrt{q} \right\}. \]

Therefore (see (3.1), (3.2) and (3.3))

\[ \Gamma_6 = \Omega A_H \Omega = \begin{bmatrix} A & B \\ B & O_3 \end{bmatrix}, \]

with

\[ A = \Omega_1 A_1 \Omega_1 = \begin{bmatrix} 0 & \frac{1}{\sqrt{p+1}\sqrt{n-p-q-1}} \\ \frac{1}{\sqrt{p+1}\sqrt{n-p-q-1}} & 0 \end{bmatrix}, \]

and

\[ B = \Omega_1 \Omega_2 = \begin{bmatrix} \frac{1}{\sqrt{p+1}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{n-p-q-1}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{q+1}} \end{bmatrix}. \]

By Theorem 3.3, as

\[ \lambda^2 I_3 - \lambda A - B^2 = \begin{bmatrix} \lambda^2 - \frac{p}{p+1} & -\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} & 0 \\ -\frac{\lambda}{\sqrt{n-p-q-1}} & \lambda^2 - n-p-q-3 & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \\ 0 & -\frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} & \lambda^2 - \frac{q}{q+1} \end{bmatrix}, \]

\[ \det(\lambda^2 I_3 - \lambda A - B^2) = \]

\[ = \left( \lambda^2 - \frac{p}{p+1} \right) \det \left( -\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} - \frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \right) \]

\[ + \left( \frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} \right) \det \left( -\frac{\lambda}{\sqrt{p+1}\sqrt{n-p-q-1}} - \frac{\lambda}{\sqrt{q+1}\sqrt{n-p-q-1}} \right) \]

\[ = \left( \lambda^2 - \frac{p}{p+1} \right) \left[ \left( \lambda^2 - \frac{n-p-q-3}{n-p-q-1} \right) \left( \lambda^2 - \frac{q}{q+1} \right) - \frac{\lambda^2}{(q+1)(n-p-q-1)} \right] \]

\[ - \left( \frac{\lambda^2}{(p+1)(n-p-q-1)} \right) \left( \lambda^2 - \frac{q}{q+1} \right) \]

\[ = \frac{(\lambda^2(p+1) - p) \left[ (\lambda^2(n-p-q-1) - (n-p-q-3))(\lambda^2(q+1) - \lambda^2) - \lambda^2 (\lambda^2(q+1) - q) \right]}{(p+1)(q+1)(n-p-q-1)}. \]
After some algebraic manipulation on the above expression, we get that

\[
\det(\lambda^2 I_3 - \lambda A - B^2) = \frac{1}{(p + 1)(q + 1)(n - p - q - 1)} \left[ (p + 1)(q + 1)(n - p - q - 1) \lambda^6 
\right.
\]

\[
- [(n - p - q - 2)(q(2p + 1) + p) + (p + 1)(q + 1)(n - p - q - 1)] \lambda^4
\]

\[
+ [pq(n - p - q - 3) + (n - p - q - 2)(q(2p + 1) + p)] \lambda^2 - pq(n - p - q - 3)
\]

\[
= \lambda^2 - 1 \left[ \eta(n, p, q) \lambda^4 - \zeta(n, p, q) \lambda^2 + \chi(n, p, q) \right]
\]

being

\[
\begin{cases}
\eta(n, p, q) &= (p + 1)(q + 1)(n - p - q - 1), \\
\zeta(n, p, q) &= (n - p - q - 2)(q(2p + 1) + p) \\
\chi(n, p, q) &= pq(n - p - q - 3).
\end{cases}
\]  

(4.1)

When obtaining the roots of the biquadratic equation

\[
\eta(n, p, q) \lambda^4 - \zeta(n, p, q) \lambda^2 + \chi(n, p, q) = 0,
\]

we determinate the roots of the equation \(\det(\lambda^2 I_3 - \lambda A - B^2) = 0\), given by:

\[
\lambda_{1,2} = \pm 1
\]

\[
\lambda_{3,4} = \pm \sqrt{\zeta(n, p, q) + \sqrt{\zeta^2(n, p, q) - 4\eta(n, p, q)\chi(n, p, q)}}
\]

\[
\lambda_{5,6} = \pm \sqrt{\zeta(n, p, q) - \sqrt{\zeta^2(n, p, q) - 4\eta(n, p, q)\chi(n, p, q)}}.
\]
Using the notation

\[
\begin{align*}
\alpha(n, p, q) &= \frac{\zeta(n, p, q)}{2n(n, p, q)}, \\
\gamma(n, p, q) &= \frac{\chi(n, p, q)}{n(n, p, q)}, \\
\beta(n, p, q) &= \sqrt{\alpha^2(n, p, q) - \gamma(n, p, q)},
\end{align*}
\] (4.2)

we get, for a general caterpillar \( T_{p,q} = T(p, n - 3 - p - q, q) \),

\[
RE(T_{p,q}) = 2 \left( 1 + \sqrt{\alpha(n, p, q) + \beta(n, p, q) + \sqrt{\alpha(n, p, q) - \beta(n, p, q)}} \right). \] (4.3)

In order to obtain the extreme graphs for certain subfamilies of caterpillar of the form \( T(p, n - p - q - 3, q) \), for \( n \geq 7 \), we consider \( q \) as a function of \( x \) such that \( 1 \leq q(x) \leq n - 5 \) for \( 1 \leq x \leq n - 5 \) and define

\[
f(x) = \sqrt{\alpha(x) + \beta(x)} + \sqrt{\alpha(x) - \beta(x)}, \] (4.4)

where \( \alpha(x) := \alpha(n, x, q(x)) \) and \( \beta(x) = \sqrt{\alpha^2(x) - \gamma(x)} := \beta(n, x, q(x)) \) as in (4.2). Therefore,

\[
f'(x) = \frac{1}{2} \left( \frac{\alpha'(x) + \beta'(x)}{\sqrt{\alpha(x) + \beta(x)}} + \frac{\alpha'(x) - \beta'(x)}{\sqrt{\alpha(x) - \beta(x)}} \right)
\]

\[
= \frac{1}{2} \left( f(x)\alpha'(x) + (\sqrt{\alpha(x) - \beta(x)} - \sqrt{\alpha(x) + \beta(x)})\beta'(x) \right) \right) \right) \right)
\]

\[
= \frac{1}{2} \left( f'(x)\alpha'(x) - 2\beta(x)\beta'(x) \right) \right) \right) \right)
\]

\[
= \frac{\alpha'(x) (f'(x) - 2\alpha(x)) + \gamma'(x)}{2f(x)\sqrt{\gamma(x)}}
\]

\[
= \frac{2\alpha'(x)\sqrt{\gamma(x)} + \gamma'(x)}{2f(x)\sqrt{\gamma(x)}},
\]

where, \( \gamma(x) := \gamma(n, x, q(x)) \). So,

\[
f'(x) \geq 0 \quad \text{if and only if} \quad \lambda(x) := 2\alpha'(x)\sqrt{\gamma(x)} + \gamma'(x) \geq 0. \] (4.5)

Taking into account (4.1) and (4.2), it is easy to see that \( 0 \leq \gamma(x) < 1 \), for all \( 1 \leq x \leq n - 5 \).

Thus,

i. If \( \alpha'(x) \geq 0 \) and \( \gamma'(x) \leq 0 \), for \( x \in I \subset [1, n - 5] \), then by (4.5)

\[
\gamma'(x) \leq \lambda(x) < 2\alpha'(x). \] (4.6)

ii. If \( \alpha'(x) \leq 0 \) and \( \gamma'(x) \geq 0 \), for \( x \in I \subset [1, n - 5] \), then by (4.5)

\[
2\alpha'(x) < \lambda(x) \leq \gamma'(x). \] (4.7)

Next we characterize the extremal caterpillars \( T(p, n - 2p - 3, q) \) for three specific cases: \( q = p \), \( q = n - p - b - 3 \) and \( q = b \), for any \( b \in \{1, \ldots, n - 6\} \) fixed.
4.2.1 Extremal graphs for the family of caterpillars $T(p, b, n - p - b - 3)$

![Diagram of caterpillar graph]

**Theorem 4.2** Let $T_p = T(p, b, n - p - b - 3)$ be a caterpillar of order $n \geq 7$, with $b \in \{1, \ldots, n-6\}$ fixed and $p = 1, \ldots, n - b - 4$. Then

$$RE(T_1) \leq RE(T_p) \leq RE\left(T_{\lfloor \frac{n-b-3}{2} \rfloor}\right).$$

**Proof** Without loss of generality, we take $1 \leq p \leq \lfloor \frac{n-b-3}{2} \rfloor$, since for $p = 1, \ldots, n - b - 4$, $T_p$ and $T_{n-p-b-3}$ are isomorphic graphs. Replacing $q$ by $n - p - b - 3$ in (4.3), and considering the function $f(x)$, as in (4.4), for $1 \leq x \leq \frac{n-b-3}{2}$,

$$\alpha'(x) = \frac{(b+1)(n-b-1)(n-2x-b-3)}{2(b+2)((x+1)(n-x-b-2))^2},$$

$$\gamma'(x) = \frac{b(n-b-2)(n-2x-b-3)}{(b+2)(x+1)^2(n-x-b-2)^2}.$$

we have both $\alpha'(x) \geq 0$ and $\gamma'(x) \geq 0$ if and only if $1 \leq x \leq \frac{n-b-3}{2}$. Thus, by (4.5), $f$ increases in the interval $[1, \frac{n-b-3}{2}]$ and the proof is complete. \qed

4.2.2 Extremal graphs for the family of caterpillar $T(p, n - 2p - 3, p)$

![Diagram of caterpillar graph]

**Theorem 4.3** Let $T_p = T(p, n - 2p - 3, p)$ be a caterpillar of order $n \geq 7$, with $p = 1, \ldots, \lfloor \frac{n-4}{2} \rfloor$. Then

$$RE(T_1) \leq RE(T_p) \leq RE(T_z),$$

where $z$ is an integer number in $I = [\text{round}(r), \text{round}(s)]$, with

$$r = \frac{1}{2} \left(2n-3-\sqrt{2n(n-2)+3}\right) \quad \text{and} \quad s = \frac{1}{2} \left(2(n-1)-\sqrt{2n(n-1)}\right).$$
Proof From (4.3), replacing $q$ by $p$, consider (see (4.4)) $f(x)$ for $1 \leq x \leq \frac{n-4}{2}$. The derivatives of $\alpha$ and $\gamma$ are
\[
\alpha'(x) = \frac{2x^2 - (4n-4)x + n^2 - 3n + 2}{(x+1)^2(n-2x-1)^2}
\]
and
\[
\gamma'(x) = \frac{2x(2x^2 - (4n-6)x + n^2 - 4n + 3)}{(x+1)^3(n-2x-1)^2}
\]
thus, we have $\alpha'(x) \geq 0$ if only if $2x^2 - (4n-4)x + n^2 - 3n + 2 \geq 0$ which occurs for $x \leq s_1$ or $x \geq s_2$ with $s_{1,2} = \frac{1}{2} \left(2(n-1) \mp \sqrt{2n(n-1)}\right)$.

Similarly, $\gamma'(x) \geq 0$ if only if $x(2x^2 - (4n-6)x + n^2 - 4n + 3) \geq 0$, that is, for $0 \leq x \leq r_1$ or $x \geq r_2$ with $r_{1,2} = \frac{1}{2} \left(2n-3 \mp \sqrt{2n(n-2)+3}\right)$.

We have $1 < r_1 < s_1 < \frac{n-4}{2} < r_2, s_2$. Therefore (see (4.5), (4.6) and (4.7)), $f$ increases in the interval $[1, r_1]$ and decreases in $[s_1, \frac{n-4}{2}]$. By Bolzano’s Theorem, there exists $z \in (r_1, s_1)$ such that $f'(z) = 0$. Since $s_1 - r_1 < 0.5$, we take $z = \text{round}(z) \in [\text{round}(r), \text{round}(s)]$, where $r = r_1$ and $s = s_1$. Finally, $f(1) < f(\frac{n-4}{2})$, so $f(1)$ is the minimum of this function. \qed

Example 1 A table with some values for $RE(T_{z-1})$, $RE(T_z)$, $RE(T_{z+1})$ and extremal caterpillars $T(p, n-3-2p, p)$ are presented below.

| $n$  | $r$    | $s$  | $z$    | $RE(T_{z-1})$ | $RE(T_z)$ | $RE(T_{z+1})$ | extremal graph |
|------|--------|------|--------|--------------|-----------|--------------|----------------|
| 19   | 4.762261 | 4.923303 | 5     | 5.388854    | 5.406881  | 5.363498     | $T(5, 6, 5)$   |
| 21   | 5.349028 | 5.508623 | 5     | 5.421848    | 5.458735  | 5.455208     | $T(5, 8, 5)$   |
| 35   | 9.453171 | 9.607738 | 10    | 5.672191    | 5.672395  | 5.662869     | $T(10, 12, 10)$|
| 50   | 13.84816 | 14.000000| 14    | 5.768798    | 5.770572  | 5.768229     | $T(14, 19, 14)$|

4.2.3 Extremal graphs of the family of caterpillars $T(p, n-p-b-3, b)$

\[
\begin{array}{c}
1 \\
\ldots \\
p \\
| n-p-b-3 | \\
\ldots \\
3 \\
\ldots \\
\ldots \\
b
\end{array}
\]

Theorem 4.4 Let $T_p = T(p, n-p-b-3, b)$ be a caterpillar of order $n \geq 7$, with $b \in \{1, \ldots, n-6\}$ fixed and $p = 1, \ldots, n - b - 4$. Then,
\[
RE(T_{n-b-4}) \leq RE(T_p) \leq RE(T_2), \text{ where } z \in I = [\text{round}(r), \text{round}(s)],
\]
with
\[
r = -(n-b-1) + \sqrt{2(n-b-1)(n-b-2)}
\]
and
\[
s = \frac{1}{b} \left( -((b+1)(n-b)-1) + \sqrt{(b+1)(n-b-1)((2b+1)(n-1)-2b^2)} \right).
\] (4.9)

**Proof** Replacing \( q \) by \( b \) in (4.3), we define \( f(x) \) as in (4.4) for \( 1 \leq x \leq n - b - 4 \). We compute
\[
\alpha'(x) = \frac{-bx^2 - 2((b+1)(n-b)-1)x + (b+1)n^2 - (b+1)(2b+3)n + b(b+2)^2 + 2}{2(b+1)((x+1)(n-x-b-1))^2},
\]
\[
\gamma'(x) = \frac{b(-x^2 - 2(n-b-1)x + n^2 - 2(b+2)n + (b+3)(b+1))}{(b+1)((x+1)(n-x-b-1))^2}.
\]

We have \( \alpha'(x) \geq 0 \) if only if \( s_1 \leq x \leq s_2 \) with
\[
s_{1,2} = \frac{1}{b} \left( -((b+1)(n-b)-1) \mp \sqrt{(b+1)(n-b-1)((2b+1)(n-1)-2b^2)} \right),
\]
and \( \gamma'(x) \geq 0 \) if only if \( r_1 \leq x \leq r_2 \) with
\[
r_{1,2} = -(n-b-1) \mp \sqrt{2(n-b-1)(n-b-2)}.
\]

We have \( 1 < r_2 < s_2 < n - b - 4 \). So, for \( s = s_2 \) and \( r = r_2 \), we get that (see (4.5), (4.6) and (4.7)) \( f \) is increasing in \([1, r]\) and decreasing in \([s, n-b-4]\). Therefore, there exists \( \bar{z} \in (r, s) \) such that \( f'({\bar{z}}) = 0 \). So, we take \( z = \text{round}({\bar{z}}) \in I = [\text{round}(r), \text{round}(s)] \). Furthermore, \( f(n-b-4) < f(1) \), which completes the proof. \( \square \)

**Example 2** To obtain the maximal Randić energy caterpillar graphs \( T(p_1, p_2, p_3) \) of order \( n = 33 \), we apply Theorems 5, 6 and 7, for slight different values of \( b \), shown in the following table.

| Theorem | \( b \) | \( r \) | \( s \) | \( z \) | \( RE(T_z) \) | extremal graph |
|---------|--------|-------|-------|-------|-------------|--------------|
| 4.2     | 12     |       | 9     | 5.653986727 | \( T(9, 12, 9) \) |
| 4.2     | 9      |       | 10    | 5.639354482 | \( T(10, 9, 11) \) |
| 4.3     | 9      | 8.867059 | 9.021749 | 9 | 5.653986727 | \( T(9, 12, 9) \) |
| 4.4     | 9      | 8.811947 | 9.031236 | 9 | 5.653986727 | \( T(9, 12, 9) \) |
| 4.4     | 8      | 9.226495 | 9.469988 | 9 | 5.652375900 | \( T(9, 13, 8) \) |
| 4.4     | 10     | 8.397368 | 8.597041 | 9 | 5.651878107 | \( T(8, 12, 10) \) |

**Remark 2** In Theorem 4.4, we find a estimated interval
\[
I = [\text{round}(r), \text{round}(s)],
\]
where \( r \) and \( s \) are given in (4.8) and (4.9), respectively, which contains the value of \( z \) that maximizes Randić energy for the family of caterpillars \( T_p = T(p, n-p-b-3, b) \), \( n \geq 7 \), with \( b \in \{1, \ldots, n-6\} \) fixed, for each \( p = 1, \ldots, n-b-4 \). In this case, we want to point out that the interval \( I \) does not necessarily has range less than 1. In fact, that interval have length less than 1 if and only if
\[
g(n,b) = 8(n+b-1)^2(n-b-1)(n-b-2) - (3n^2 - 3bn - 9n + 2b + 6)^2 > 0,
\]
and this function $g(n, b)$ can be written as:

$$g(n, b) = 8(n + b - 1)^2(n - b - 1)(n - b - 2) - \left(3(n - 1)(n - 2) - (3n - 2)b\right)^2.$$ 

Since $n - b - 1 > n - b - 2 > 0$ then $g(n, b) > h(n, b)$, with

$$h(n, b) = 8(n + b - 1)^2(n - b - 2)^2 - \left(3(n - 1)(n - 2) - (3n - 2)b\right)^2$$

$$= \left(\sqrt{8}(n + b - 1)(n - b - 2) - 3(n - 1)(n - 2) + (3n - 2)b\right)$$

$$\times \left(\sqrt{8}(n + b - 1)(n - b - 2) + 3(n - 1)(n - 2) - (3n - 2)b\right).$$

For each $n$, we find the values of $b$ such that

$$\Delta_1 = \sqrt{8}(n + b - 1)(n - b - 2) - 3(n - 1)(n - 2) + (3n - 2)b > 0,$$

and,  

$$\Delta_2 = \sqrt{8}(n + b - 1)(n - b - 2) + 3(n - 1)(n - 2) - (3n - 2)b > 0.$$ 

Taking into account that $3n - 2 > 3(n - 1) > 0$, then

$$\Delta_1 > \sqrt{8}(n + b - 1)(n - b - 2) - 3(n - 1)(n - 2) + 3(n - 1)b$$

$$= \left(\sqrt{8}b - (3 - \sqrt{8})(n - 1)\right)(n - b - 2).$$

Since

$$\sqrt{8}b - (3 - \sqrt{8})(n - 1) > 0 \iff b > \frac{(3 - \sqrt{8})}{\sqrt{8}}(n - 1) \approx 0.06066(n - 1),$$

for such values of $b$, $\Delta_1 > 0$. Now, let us show that

$$\Delta_2 = \sqrt{8}(n + b - 1)(n - b - 2) - (3n - 2)b + 3(n - 1)(n - 2) > 0.$$ 

From

$$-(3n - 2)b + 3(n - 1)(n - 2) > 0 \iff b < \frac{3(n - 1)(n - 2)}{3n - 2}$$

and

$$n - 6 < \frac{3(n - 1)(n - 2)}{3n - 2} \iff 3n^3 - 20n + 12 < 3(n^2 - 3n + 2) \iff 6 < 11n \quad \text{(which is true),}$$

it follows that $\Delta_2 > 0$, for $1 \leq b \leq n - 6 < \frac{3(n - 1)(n - 2)}{3n - 2}$.

From the above, for $n \geq 7$ and $b \in \mathbb{N}$ such that $0.06066(n - 1) \leq b \leq n - 6$,

$$g(n, b) > h(n, b) = \Delta_1 \Delta_2 > 0.$$
Given \( n \geq 7 \), consider \( b_{\text{min}} \) the smallest integer \( b \geq 1 \) such that \( g(n,b) > 0 \) and let \( b^* = 0.06066(n - 1) \). For different values of \( n \), \( b^* \) remains close to the exact value \( b_{\text{min}} \):

| \( n \)  | \( b_{\text{min}} \) | \( b^* \) |
|-------|----------------|-------|
| 20    | 1              | 1.1525|
| 30    | 2              | 1.7591|
| 50    | 3              | 2.9723|
| 100   | 6              | 6.0053|
| 500   | 30             | 30.269|
| 1000  | 61             | 60.599|
| 5000  | 303            | 303.24|
| 10000 | 606            | 606.54|
| 20000 | 1213           | 1213.1|

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Domingos M. Cardoso
Department of Mathematics
Universidade de Aveiro
Aveiro, Portugal
E-mails: dcardoso@ua.pt

Paula Carvalho
Department of Mathematics
Universidade de Aveiro
Aveiro, Portugal
E-mails: paula.carvalho@ua.pt

Roberto C. Díaz
Departamento de Matemáticas,
Universidad de La Serena
La Serena, Chile
E-mails: roberto.diazm@userena.cl

Paula Rama
Department of Mathematics
Universidade de Aveiro
Aveiro, Portugal
E-mails: prama@ua.pt