Upper bound for the energy of the starlike trees

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Abstract. The energy graph was defined by Gutman, in 1978, as the sum of the absolute values of the eigenvalues of the adjacency matrix. In this work, we obtain a upper bound for the energy of a starlike tree. This bound is obtained in function of the number of vertices and the maximum degree of the vertices.

1. Introduction and preliminaries
Let $G$ be a simple undirected graph on $n$ vertices and $m$ edges. The spectrum of a simple undirected graph are the eigenvalues of the $(0, 1)$-adjacency matrix of graph. We observe that the adjacency matrix is a real symmetric matrix, then the eigenvalues of adjacency matrix are real numbers and we can denote $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Moreover, if $G$ is a connected graph, then the adjacency matrix is an irreducible matrix, so the spectral radius is the largest eigenvalue and this eigenvalue has simple multiplicity.

Connected simple undirected graphs are of great interest in molecular topology, a field of chemistry which reduces the molecule to a connected simple undirected graph. Eigenvalues and characteristic polynomial have found their use in the characterization of chemical compounds. On applications of eigenvalues, characteristic polynomial and graph invariants to chemistry, we mention the works in [3, 4, 14, 15].

A tree is a connected acyclic graph and a tree is called starlike if exactly one of its vertices has degree greater than two [19]. In this class of trees, one can choose as the root vertex the vertex with the greatest degree. A starlike tree can be denoted by $S(n_1, n_2, \ldots, n_k)$, where $n_i$ is the number of vertices in the $i$-th branch obtained by eliminating the root vertex of the starlike tree. Without loss of generality, we can assume that $n_1 \geq n_2 \geq \cdots \geq n_k$.

Example 1 The following figure shows the starlike tree $S(6, 4, 4, 3, 2, 1, 1)$
We recall that the spectrum of a simple undirected graph are the eigenvalues of the adjacency matrix $A(G)$. In this case, the adjacency matrix is a real symmetric matrix and it has real eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The largest eigenvalue $\lambda_1$ is called the spectral radius, or the index, of the graph. The eigenvalues of the adjacency matrix are known as the eigenvalues of the graph, and the characteristic polynomial of $\phi(G, x) = \det (xI - A(G))$ is the characteristic polynomial of the graph $G$, where $I$ is the identity matrix of appropriate order.

For a simple undirected graph $G$ on $n$ vertices with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, Gutman, in 1978, defined the energy of the graph, $E(G)$, as the sum of the absolute value of its eigenvalues [5], that is

$$E(G) = \sum_{i=1}^{n} |\lambda_i|. \quad (1)$$

The concept of graph energy appears in chemistry where certain numerical quantities, such as the heat of formation of a hydrocarbon, are related to total $\pi$-electron energy that can be calculated as the energy of an appropriate molecular graph (see [6]).

Several authors have studied the energy of a graph and in many cases it is not possible to determine exactly the energy of the graph, therefore a research problem is to obtain bounds for the energy. In some cases, particular graphs are studied, for example the energy of bipartite graphs, cyclic and acyclic graphs, regular graph (see, e.g., [2, 7, 9, 10, 16, 17, 18]). About the problem of obtaining bounds of the energy graphs, some bounds are given in terms of $n$ (number of vertices) and $m$ (number of edges). Previously, in 1970 McClelland [13] obtained a bound for the sum of the absolute value of the eigenvalues of a Hermitian matrix in terms of the number of vertices and the Frobenius norm of the matrix.

We recall that the Frobenius norm of an $n \times n$ matrix $M = (m_{i,j})$ is

$$\|M\| = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} |m_{i,j}|^2}. $$

Thus, the bound given by McClelland, in terms of $n$ and $m$ is show in the following theorem.

**Theorem 1** [13] Let $G$ be a graph on $n$ vertices and $m$ edges. Then

$$E(G) \leq \sqrt{2mn}. $$

Other bound in terms of $n$ and $m$ is given by Koolen and Moulton in 2001.
Theorem 2 [11] If \( 2m \geq n \) and \( G \) is a graph on \( n \) vertices with \( m \) edges, then the inequality
\[
E(G) \leq \frac{2m}{n} + \sqrt{(n-1) \left[ 2m - \left( \frac{2m}{n} \right)^2 \right]}
\]
holds. Moreover, equality holds if and only if \( G \) is either \( \frac{3}{2}K_2 \), \( K_n \), or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value
\[
\sqrt{\left(2m - \left( \frac{2m}{n} \right)^2 \right) / (n-1)}.
\]

Different bounds for the energy of a graph have been obtained over time, but not all expressions (of bounds) have the same level of implementation difficulty. For more details on graph energy, see [8, 12]).

In this work we obtain a bound for the energy of a Starlike tree in terms of the greatest degree of its vertices. To finish this Section, we recall a result on the spectral radius of a Starlike tree, which will be important in obtaining our result.

Theorem 3 [1] Let \( \lambda_1 \) be the largest eigenvalue of the starlike tree \( S(n_1, n_2, \ldots, n_k) \), where \( n_1 \geq n_2 \geq n_3 \geq \cdots \geq n_k \) and \( n_3 > 1 \). Then
\[
\frac{k-1}{\sqrt{k-2}} < \lambda_1.
\]

2. Upper bound for the Energy of the Starlike trees
In this Section we obtain the main result. Previously, we need to prove the following Lemmas.

Lemma 1 Let \( S(n_1, n_2, \ldots, n_k) \) be a starlike tree, with \( n_3 > 1 \) and \( m \) edges. Then
\[
\sqrt{\frac{2m}{n}} < \frac{k-1}{\sqrt{k-2}}.
\]

Proof. We recall that for every tree \( m = n - 1 \geq 0 \). Then
\[
\sqrt{\frac{2m}{n}} \leq \frac{2m}{n} = 2 - \frac{2}{n} < 2.
\]

On the other hand, we observe that if \( n_3 > 1 \), then \( k \geq 3 \). Thus \( k - 2 > 0 \) and \( k - 1 > 0 \). Now, it is easy to see that
\[
2 \leq \frac{k-1}{\sqrt{k-2}} \quad \text{if and only if} \quad (k-3)^2 \geq 0.
\]

Therefore the result is proved.

Lemma 2 Let \( S(n_1, n_2, \ldots, n_k) \) be a starlike tree, with \( n_3 > 1 \) and \( m \) edges. Then
\[
\frac{k-1}{\sqrt{k-2}} < \sqrt{2m}.
\]

Proof. Let \( T_{k+1} \) be a star tree with \( k \) pendent vertices. We observe that \( T_{k+1} \) is a subgraph of \( S(n_1, n_2, \ldots, n_k) \), then \( k < m \). Now, prove that \( \frac{k-1}{\sqrt{k-2}} < \sqrt{2k} \) is equivalent to prove that
\[
3k^2 - 2k - 1 > 0.
\]

This last expression is true for all \( k > 1 \). Therefore, we obtain
\[
\frac{k-1}{\sqrt{k-2}} < \sqrt{2k} < \sqrt{2m}.
\]
**Theorem 4** Let \( S(n_1, n_2, \ldots, n_k) \) be a starlike tree, with \( n_3 > 1 \). Then,

\[
E(S(n_1, n_2, \ldots, n_k)) < \frac{k - 1}{\sqrt{k - 2}} + \sqrt{(n - 1) \left(2(n - 1) - \frac{(k - 1)^2}{k - 2}\right)}
\]

**Proof.** Following the techniques used by Koolen and Moulton, from Equation (1), we can write

\[
E(G) - \lambda_1 = \sum_{i=2}^{n} |\lambda_i|
\]

and using the Cauchy–Schwarz inequality, we obtain

\[
(E(G) - \lambda_1)^2 \leq (n - 1) \sum_{i=2}^{n} (\lambda_i)^2.
\]

Then

\[
E(G) \leq \lambda_1 + \sqrt{(n - 1) \left(\sum_{i=1}^{n} (\lambda_i)^2 - (\lambda_1)^2\right)}.
\]

Now, we recall that for the adjacency matrix we have \( \sum_{i=1}^{n} (\lambda_i)^2 = 2m \). Then

\[
E(G) \leq \lambda_1 + \sqrt{(n - 1)(2m - (\lambda_1)^2)}.
\]

We observe that \( f(x) = x + \sqrt{(n - 1)(2m - x^2)} \) is a decreasing function in the variable \( x \in \left[\sqrt{2m/n}, \sqrt{2m}\right] \). From Lemma 1 and Lemma 2 we obtain the following inequalities for the bound given in Theorem 3

\[
\sqrt{\frac{2m}{n}} < \frac{k - 1}{\sqrt{k - 2}} < \sqrt{2m}.
\]

Then \( E(S(n_1, \ldots, n_k)) < f \left(\frac{k - 1}{\sqrt{k - 2}}\right) \). Since every tree has \( n - 1 \) edges, the result is obtained. 

**Example 2** The following table shows some examples of the bounds stated in the previous theorems, the results are given to four decimal places.

| \( S(n_1, \ldots, n_k) \) | \( E(S(n_1, \ldots, n_k)) \) | Theorem 4 | Theorem 2 | Theorem 1 |
|---------------------------|-----------------|-----------|-----------|-----------|
| \( S(2, 2, 2) \)         | 8               | 8,9282    | 9,0877    | 9,1652    |
| \( S(4, 3, 2) \)         | 11,9669         | 13,2250   | 13,3256   | 13,4164   |
| \( S(10, 8, 7) \)        | 32,2708         | 35,9116   | 35,9458   | 36,0555   |
| \( S(10, 10, 10) \)      | 51,1450         | 57,0758   | 57,1573   | 57,2713   |
| \( S(2, 2, 2) \)         | 10,4721         | 11,7130   | 11,9127   | 12        |
| \( S(6, 5, 4, 3, 2) \)   | 25,3841         | 28,6406   | 28,8758   | 28,9828   |
| \( S(7, 6, 5, 4, 3, 2) \)| 37,8265         | 38,4061   | 38,7739   | 38,8844   |
| \( S(3, 3, 3, 3, 3, 3, 3)\) | 24,5314       | 29,7166   | 30,2898   | 30,3974   |
| \( S(5, 5, 4, 4, 3, 3, 2, 2) \) | 34,3217     | 39,4546   | 40,1879   | 40,2989   |
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