On the sum of the Laplacian eigenvalues of a tree
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1. Introduction

For a simple graph $G$ with vertex set $V = \{v_1, \ldots, v_n\}$ and adjacency matrix $A$, the Laplacian spectrum of $G$ is the set of eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ of the Laplacian matrix of $G$, given by $L = D - A$, where $D$ is the diagonal matrix of vertex degrees of $G$.

The present paper considers the sum $S_k(G) = \sum_{i=1}^{k} \mu_i$ of the $k$ largest Laplacian eigenvalues of a graph $G$. A conjecture by Brouwer [2] states that, given a graph $G = (V, E)$ with $n$ vertices and an integer $k \in \{1, \ldots, n\}$, the sum $S_k(G)$ satisfies

$$S_k(G) \leq |E| + \binom{k+1}{2}.$$

For $k = 1$, the conjecture follows from the well-known inequality $\mu_1(G) \leq |V(G)|$, and the cases $k = n$ and $k = n - 1$ are also straightforward. Haemers et al. [5] established that this conjecture also
holds for \( k = 2 \). Moreover, they proved that, if \( T \) is a tree with \( n \) vertices and \( 1 \leq k \leq n \), then the sum \( S_k(T) \) is bounded by

\[
S_k(T) \leq (n - 1) + 2k - 1, \quad \text{for} \quad 1 \leq k \leq n, \tag{1}
\]

which implies that Brouwer’s conjecture is correct for trees in general. In a similar direction, Zhou [14] has considered the sum of powers of the Laplacian eigenvalues of a graph.

In this work, we also study the sum \( S_k(T) = \sum_{i=1}^{k} \mu_i \) of the largest Laplacian eigenvalues of a tree \( T \). More precisely, we improve the upper bound in (1) for every \( k > 1 \), proving the following result.

**Theorem 1.1.** Let \( T \) be a tree with \( n \) vertices and let \( 1 \leq k \leq n \). Then the sum \( S_k(T) \) of the \( k \) largest Laplacian eigenvalues of \( T \) satisfies

\[
S_k(T) \leq (n - 1) + 2k - 1 - \frac{2k - 2}{n} \tag{2}
\]

Moreover, equality is achieved only when \( k = 1 \) and \( T \) is a star on \( n \) vertices.

Note that this upper bound is not tight unless \( k = 1 \), in which case it coincides with the upper bound in (1). However, it is easy to see that, for \( k \geq 2 \), this bound may not be improved by a factor of \( 1/n \). Indeed, if \( k = 2 \) and \( T = P_4 \) is the path on four vertices, it is well known that

\[
S_2(P_4) = 4 + \sqrt{2} > 5.25 = 3 + 2 \cdot 2 - 1 - \frac{2 \cdot 2 - 1}{4}.
\]

Furthermore, Theorem 1.1 allows us to prove that, among all trees with \( n \) vertices, the star has the highest Laplacian energy, which was conjectured by Radenković and Gutman [10].

### 1.1. Application to Laplacian energy

Given a graph \( G \) with \( n \) vertices and average degree \( \bar{d} \), the Laplacian energy of \( G \), first defined by Gutman and Zhou [4], is given by

\[
LE(G) = \sum_{i=1}^{n} |\mu_i - \bar{d}|.
\]

For more details on the Laplacian energy see [15] and the references cited therein.

Several open problems in spectral graph theory have an extremal nature. They may involve finding the extremal value of some spectral parameter over a class of graphs, characterizing the elements of this class that achieve this extremal value, or even ordering the elements in this class according to the value of this parameter. As an illustration, the connected graphs on \( n \)-vertex with smallest/highest Laplacian energy are not known for general \( n \), not even when the class is restricted to trees.

On the other hand, more is known if the spectral parameter under consideration is the energy of a graph \( G \), which is defined as the sum \( E(G) = \sum_{i=1}^{n} |\lambda_i| \), where \( \lambda_1, \ldots, \lambda_n \) are the eigenvalues of the adjacency matrix of \( G \). Indeed, if \( P_n \) and \( S_n \) stand for the \( n \)-vertex path and the \( n \)-vertex star, respectively, the following bounds hold.

**Theorem 1.2 (Gutman [3]).** Let \( T \) be a tree on \( n \) vertices. Then

\[
E(S_n) \leq E(T) \leq E(P_n).
\]

Radenković and Gutman [10] studied the correlation between the energy and the Laplacian energy of trees. Among other things, they computed the energy and the Laplacian energy for all trees up to 14 vertices. Their experiments suggest that, for trees, energy and Laplacian energy behave very differently. In particular, they formulated the following conjecture.


Conjecture 1. Let $T$ be a tree on $n$ vertices. Then
\[ LE(P_n) \leq LE(T) \leq LE(S_n). \]

In a recent paper by Trevisan et al. [12], it has been shown that the conjecture is true for trees of diameter 3. We now show that the upper bound in Conjecture 1 is an easy consequence of Theorem 1.1.

Theorem 1.3. Let $T$ be a tree on $n$ vertices such that $T \neq S_n$. Then it holds that
\[ LE(T) < LE(S_n). \]

Proof. It is well known that the Laplacian spectrum of $S_n$ is \{0, 1, $n - 2$, $n\}$, hence, using that $d = 2 - \frac{2}{n}$, we have
\[ LE(S_n) = \bar{d} + (\bar{d} - 1)(n - 2) + (n - \bar{d}) = 2n - 4 + \frac{4}{n}. \]

Let $T$ be an $n$-vertex tree that is not a star and has Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. Let $\sigma$ be the number of Laplacian eigenvalues larger than the average degree $d$ of $T$. Note that the quantity $n\bar{d}$ is equal to the trace of the Laplacian matrix of $T$, which in turn is the sum of the vertex degrees of $T$. This leads to $\bar{d} = \frac{2}{n} \cdot |E| = 2 - \frac{2}{n}$, and implies that the Laplacian energy of $T$ is given by
\[ LE(T) = \sum_{i=1}^{n} |\mu_i - \bar{d}| = \sum_{i=1}^{\sigma} (\mu_i - \bar{d}) + \sum_{i=\sigma+1}^{n} (\bar{d} - \mu_i) = (n - 2\sigma)\bar{d} + \sum_{i=1}^{\sigma} \mu_i - \sum_{i=\sigma+1}^{n} \mu_i = (n - 2\sigma)\bar{d} - \sum_{i=1}^{n} \mu_i + 2\sum_{i=1}^{\sigma} \mu_i < (n - 2\sigma)\bar{d} - n\bar{d} + 2 \left[ n - 1 + 2\sigma - 1 - \frac{2\sigma - 2}{n} \right] \]
\[ = 2n - 4 + \frac{4}{n}, \]
proving the result. Notice that we used Theorem 1.1 to establish (3). □

In order to give an overview of the structure of this paper, we briefly discuss the main aspects of the proof of Theorem 1.1. It relies on several ingredients from other papers, which are described in Section 2. Moving to the proof, the first observation is that it is sufficient to prove the theorem in the case $k = \sigma$, where $\sigma$ is the number of Laplacian eigenvalues of the tree $T$ that are larger than their average value $\bar{d}$ (see Lemma 3.1). This simplified version is then proved for all trees in two general steps. At first, one shows that the theorem holds for some special families of trees. In Section 3, this is done for stars and for trees $T$ that can be split into two nontrivial stars by the removal of an edge. A more elaborate case is the subject of Sections 4 and 5. In these two sections, we are interested in trees $T$ such that, for every edge $e$ in $T$ whose endpoints are not leaves, the deletion of $e$ yields a star and a tree with diameter at least three (that is, a non-star). Finally, to extend the bound in the statement of Theorem 1.1 from these special families to the general case, one uses induction. This inductive step is addressed in Section 6.

2. Preliminaries

In this section, we discuss auxiliary results that will be used in the proof of Theorem 1.1. The main tools are a decomposition result, which estimates the spectrum of a matrix based on a decomposition of this matrix as a sum of matrices, and an eigenvalue localization algorithm, which determines the number of eigenvalues of a tree in a given interval. Another important ingredient in our proofs is
a characterization of the Laplacian spectrum of a particular family of trees, which was obtained by Rojo [11] and will be discussed in Section 4.

Given a real symmetric matrix $A$ of order $n$, the spectrum of $A$ is the set of $n$ real eigenvalues of $A$ (with their respective multiplicities), which are denoted in nonincreasing order by $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A)$. The following result by Wielandt [13] plays a special role in our proofs, as it gives an upper bound on the sum of any prescribed subset of eigenvalues of a symmetric matrix $A$ in terms of the eigenvalues of the matrices in any decomposition of $A$ as a sum of symmetric matrices.

**Theorem 2.1.** Let $A$, $B$, $C$ be hermitian matrices of order $n$ such that $A = B + C$. Then

$$\sum_{i \in I} \lambda_i(A) \leq \sum_{i=1}^{\vert I \vert} \lambda_i(B) + \sum_{i \in I} \lambda_i(C)$$

for every subset $I \subset \{1, 2, \ldots, n\}$.

Observe that the statement of this theorem is not symmetric for $B$ and $C$. While the same index set is used for $A$ and $C$, the eigenvalues taken from $B$ are the $\vert I \vert$ largest.

In our calculations, two bounds will prove to be particularly useful, the first being a lower bound on the smallest nonzero Laplacian eigenvalue, and the second being an upper bound on the largest Laplacian eigenvalue of every tree that is not a star.

The following is a result of McKay, whose proof was published for the first time in [9].

**Lemma 2.2.** Let $G$ be a connected $n$-vertex graph with diameter $D$ and Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. The algebraic connectivity $\mu_{n-1}$ of $G$ satisfies

$$\mu_{n-1} \geq \frac{4}{Dn}.$$ 

Now, we may use a result by Li and Zhang [8] to derive the following upper bound on the largest Laplacian eigenvalue of a tree with diameter at least three.

**Lemma 2.3.** Let be $T$ a $n$-vertex tree that is not a star. Then its largest Laplacian eigenvalue $\mu_1$ satisfies

$$\mu_1 < n - \frac{1}{2}.$$

**Proof.** The following bound on the value of the largest Laplacian eigenvalue of a graph $G$ is due to Li and Zhang (see Theorem 3.2 in [8]):

$$\mu_1 \leq 2 + \sqrt{(d_1 + d_2 - 2)(d_1 + d_3 - 2)},$$

where $d_i$ denotes the $i$th largest vertex degree in $G$.

Let $T$ be an $n$-vertex tree that is not a star. Then $d_i \geq 1$ for every $i$ and $d_2 \geq 2$. Since $\sum_{i=1}^{n} d_i = 2(n - 1)$, we have

$$d_1 + d_2 + d_3 \leq 2(n - 1) - (n - 3) = n + 1.$$

Using that $d_2 \geq 2$ and $d_3 \geq 1$, we further conclude that

$$d_1 + d_2 \leq n,$$

$$d_1 + d_3 \leq n - 1,$$

from which we obtain
\[ \mu_1 \leq 2 + \sqrt{(n-2)(n-3)} \]
\[ = 2 + \sqrt{(n - \frac{5}{2})^2 - \frac{1}{4}} \]
\[ < 2 + n - \frac{5}{2} = n - \frac{1}{2}, \]
which establishes our result. \(\square\)

To conclude this section, we describe an algorithm due to Jacobs and Trevisan [6] that can be used to estimate the Laplacian eigenvalues of a given tree. It counts the number of eigenvalues of the adjacency matrix of a tree \(T\) lying in any real interval. The algorithm is based on the diagonalization of the matrix \(A(T) + \alpha I\), where \(A(T)\) is the adjacency matrix of \(T\) and \(\alpha\) is a real number. One of the main features of this algorithm is that it can be executed directly on the tree, so that the adjacency matrix is not needed explicitly. By focusing on the diagonalization of the matrix \(L(G) + \alpha I\) instead, this algorithm can be readily adapted to calculate the number of eigenvalues of the Laplacian matrix of \(T\) lying in a given interval, as we now see (Fig. 1).

It is worth noticing that the diagonal elements of the output matrix correspond precisely to the values \(a(v)\) on each node \(v\) of the tree. The following result is going to be used throughout the paper.

**Lemma 2.4** (Jacobs and Trevisan [6]). Let \(T\) be a tree and let \(D\) be the diagonal matrix produced by the algorithm \(\text{Diagonalize}(T, -\alpha)\). The following assertions hold.

(a) The number of positive entries in \(D\) is the number of Laplacian eigenvalues of \(T\) that are greater than \(\alpha\).
(b) The number of negative entries in \(D\) is the number of Laplacian eigenvalues of \(T\) that are smaller than \(\alpha\).
(c) If there are \(j\) zero entries in \(D\), then \(\alpha\) is a Laplacian eigenvalue of \(T\) with multiplicity \(j\).

To illustrate how the algorithm performs, we look at an example. Consider the tree with diameter four in Fig. 2, where \(v_0\) is the root with children \(v_1\) and \(v_2\), each having \(s_1\) and \(s_2\) leaves, respectively. Notice that the number of nodes of the tree is \(n = s_1 + s_2 + 3\).

Input: tree \(T\), scalar \(\alpha\)
Output: diagonal matrix \(D\) congruent to \(L(T) + \alpha I\)

**Algorithm** \(\text{Diagonalize}(T, \alpha)\)
initialize \(a(v) := d(v) + \alpha\), for all vertices \(v\)
order vertices bottom up
for \(k = 1\) to \(n\)
if \(v_k\) is a leaf then continue
else if \(a(c) \neq 0\) for all children \(c\) of \(v_k\) then
    \(a(v_k) := a(v_k) - \frac{1}{a(c)}\), summing over all children of \(v_k\)
else
    select one child \(v_j\) of \(v_k\) for which \(a(v_j) = 0\)
    \(d(v_k) := -\frac{1}{2}\)
    \(d(v_j) := 2\)
    if \(v_k\) has a parent \(v_i\), remove the edge \(v_kv_i\).
end loop

**Fig. 1.** Diagonalizing \(L(T) + \alpha I\).
Lemma 2.5. The Laplacian eigenvalues of the tree of Fig. 2 satisfy the following properties:

(a) the multiplicity of 1 as an eigenvalue is \( s_1 + s_2 - 2 \);
(b) two eigenvalues are smaller than 1;
(c) three eigenvalues are greater than 1;
(d) two eigenvalues are greater than 2.

Proof. We apply the algorithm to the tree with \( \alpha = -1 \). The initialization step assigns the value zero to all leaves, whereas \( a(v_i) = s_i \) for \( i = 1, 2 \), and \( a(v_0) = 1 \). When processing vertices \( v_1 \) and \( v_2 \), we choose one leaf of each to change to the value 2, which leads to the values \( a(v_i) = -1/2 \) for \( i = 1, 2 \), and the removal of both edges between them and the root \( v_0 \). Hence \( a(v_0) = 1 \) remains unchanged and the algorithm finishes, proving items (a)–(c). This process is illustrated in Figs. 3 and 4. For item (d), we apply the algorithm with \( \alpha = -2 \). □
3. Particular cases

In this section, we shall describe families of trees for which Theorem 1.1 holds. For a tree \( T = (V, E) \) on \( n \) vertices, the Laplacian eigenvalues of \( T \) are again denoted by \( \mu_1(T) \geq \mu_2(T) \geq \cdots \geq \mu_n(T) \). As we shall see, the number of Laplacian eigenvalues larger than the average \( \overline{d} = \frac{1}{n} \sum \mu_i(T) \) plays an important role in our argument.

Let \( \sigma = \sigma(T) \) denote the number of Laplacian eigenvalues of \( T \) that are larger than \( \overline{d} \). We show that it suffices to prove Theorem 1.1 for the \( \sigma \) largest eigenvalues.

Lemma 3.1. Let \( T = (V, E) \) be a tree for which exactly \( \sigma \) Laplacian eigenvalues are larger than their average \( \overline{d} \). If the inequality

\[
S_k = \sum_{i=1}^{k} \mu_i(T) \leq |E| + 2k - 1 - \frac{2k - 2}{n}
\]

is satisfied for \( k = \sigma \), then it is satisfied for every \( k \in \{1, \ldots, n\} \). Moreover, if the inequality is strict for \( k = \sigma \), then it is strict for every value of \( k \).

Proof. Let \( 1 \leq k_1 < \sigma < k_2 \leq n \). We prove that the inequality holds for \( k_1 \) and \( k_2 \). On the one hand, since \( \mu_{\sigma} > \overline{d} = 2 - \frac{2}{n} \), we have

\[
S_{k_1} = S_{\sigma} - \sum_{i=k_1+1}^{\sigma} \mu_i(T) \\
\leq S_{\sigma} - (\sigma - k_1) \mu_\sigma(T) \\
< S_{\sigma} - (\sigma - k_1)\left(2 - \frac{2}{n}\right) \\
\leq |E| + 2\sigma - 1 - \frac{2\sigma - 2}{n} - 2(\sigma - k_1) + \frac{2\sigma - 2k_1}{n} \\
= |E| + 2k_1 - 1 - \frac{2k_1 - 2}{n}.
\]

On the other hand, by the fact that \( \mu_{\sigma+1} \leq \overline{d} = 2 - \frac{2}{n} \), it holds that

\[
S_{k_2} = S_{\sigma} + \sum_{i=\sigma+1}^{k_2} \mu_i(T) \\
\leq S_{\sigma} + (k_2 - \sigma) \mu_{\sigma+1}(T) \\
\leq S_{\sigma} + (k_2 - \sigma)\left(2 - \frac{2}{n}\right) \\
\leq |E| + 2\sigma - 1 - \frac{2\sigma - 2}{n} + 2(k_2 - \sigma) + \frac{2\sigma - 2k_2}{n} \\
= |E| + 2k_2 - 1 - \frac{2k_2 - 2}{n}.
\]

Clearly, this inequality is strict for \( k_2 \) if \( S_{\sigma} < |E| + 2\sigma - 1 - \frac{2\sigma - 2}{n} \). This concludes the proof. \( \square \)

This result can be used to establish Theorem 1.1 for some special classes of trees. One of them is the class of all stars, and the other is the class of all non-stars \( T \) such that there exists an edge \( e \) of \( T \) whose endpoints are not leaves for which the components of \( T \setminus \{e\} \) are stars. Because of this property, we call the trees in this family S&S-trees (Star–Star trees). It is easy to see that the set there are essentially three types of S&S-trees:
(i) trees with diameter three (see Fig. 5);
(ii) trees with diameter four consisting of a path on five vertices whose central vertex has degree two, while the other two nonleaf vertices may have arbitrary degree. This type of tree is often called a double broom with diameter four (see Fig. 2);
(iii) trees with diameter five consisting of a path on six vertices such that an arbitrary number of leaves may be appended to the second and the fifth vertex. This type of tree is often called a double broom with diameter five (see Fig. 6).

Lemma 3.2. Let $T = (V, E)$ be a tree on $n$ vertices with Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = 0$, and assume that $T$ satisfies one of the following:

(a) $T$ is a star;
(b) $T$ is a tree with diameter 3;
(c) $T$ is a double broom with diameter 4;
(d) $T$ is a double broom with diameter 5.

Then, for every $k \in \{1, \ldots, n\}$ it holds that

$$S_k(T) \leq \sum_{i=1}^{k} \mu_i = |E| + 2k - 1 - \frac{2k - 2}{n} = n + 2k - 2 - \frac{2k - 2}{n}.$$  

Equality holds only when $k = 1$ and $T$ is an $n$-vertex star.

Proof. If $T$ has a single vertex, the result is trivial, as its single Laplacian eigenvalue is 0. Let $T = (V, E)$ be a star on $n \geq 2$ vertices, so that it has Laplacian eigenvalues $n$ (multiplicity 1), 1 (multiplicity $n-2$) and 0 (multiplicity 1). As a consequence, we have

$$S_k(T) \leq n + k - 1 = |E| + k \leq |E| + 2k - 1 - \frac{2k - 2}{n},$$  

as required. If $k = 1$, the two inequalities in the above calculation are in fact equalities, so that the inequality in the statement of Theorem 1.1 is tight in this case. For $n = 2$, the only other possibility for $k$ is $k = 2$, for which we have

$$S_2(T) = n = 2 < 3 = |E| + 2 \cdot 2 - 1 - \frac{2 \cdot 2 - 2}{2},$$
so that the inequality is strict in this case. Finally, if \( k \geq 2 \) and \( n \geq 3 \), the second inequality in (4) is strict, as

\[
2k - 1 - \frac{2k - 2}{n} \geq 2k - 1 - \frac{2k - 2}{3} = k + \frac{k - 1}{3} > k.
\]

Now, assume that \( T \) is a tree with diameter 3 for which the two central vertices are adjacent to \( s_1, s_2 \geq 1 \) leaves, respectively. In particular, the tree \( T \) contains at least four vertices and the average of the Laplacian eigenvalues satisfies \( \bar{\lambda} = 2 - 2/n \geq 3/2 \). Following Trevisan et al. [12], the characteristic polynomial of the Laplacian matrix of \( T \) is given by

\[
p(x) = (x^2 - (n + 2)x^2 + (2n + s_1s_2 + 1)x - n) (x - 1)^{n-4}x.
\]

Moreover, the authors of [12] prove that the polynomial with degree three contains the two largest Laplacian eigenvalues \( \mu_1(T) \) and \( \mu_2(T) \), which are both greater than \( \bar{\lambda} \), while its third root is equal to the algebraic connectivity \( \mu_{n-1}(T) \) of \( T \), which is strictly larger than \( 2/n \). This implies that \( \sigma = 2 \). As a consequence, we have

\[
S_2(T) = \mu_1(T) + \mu_2(T) = n + 2 - \mu_{n-1}(T) < n + 2 - \frac{2}{n} = |E| + 2 \cdot 2 - 1 - \frac{2 \cdot 2 - 2}{n},
\]

so that (2) holds and is strict for general \( k \) by Lemma 3.1.

Now, assume that \( T = (V, E) \) is a double broom with diameter four for which the two central vertices are adjacent to \( s_1, s_2 \geq 1 \) leaves, respectively. Note that \( n \geq 5 \). One can show (for instance, adapting the algorithm of Jacobs et al. [7] to the Laplacian matrix) that the characteristic polynomial of the Laplacian matrix of \( T \) is equal to

\[
p(x) = q(x) \cdot (x - 1)^{n-5}x, \quad \text{where}
\]

\[
q(x) = x^4 - (n + 3)x^3 + (s_1s_2 + 4s_1 + 4s_2 + 12)x^2 - (2s_1s_2 + 4s_1 + 4s_2 + 10)x + n.
\]

Let \( x_1 \geq \cdots \geq x_4 \) be the roots of \( q(x) \). Applying Algorithm Diagonalize for \( \alpha = -2 \), we determine through Lemma 2.4 that \( T \) has precisely two eigenvalues that are larger than two, from which we deduce that \( x_1, x_2 > 2 \). We can also establish that \( q(x) \) has a single root smaller than 1, which satisfies \( x_4 \geq \frac{1}{n} \) in light of Lemma 2.2 (note that \( T \) has diameter \( D = 4 \)). We now estimate the remaining root of \( q(x) \). Observe that

\[
q(1) = -s_1s_2 < 0,
\]

\[
q(2) = s_1 + s_2 - 1 > 0.
\]

In addition to this, assuming that \( s_1 \geq s_2 \geq 1 \), we have

\[
q(6/5) = \frac{1}{125} (-120s_1s_2 + 29s_1 + 29s_2 - 9/5) \leq \frac{1}{125} (-120s_1s_2 + 58s_1 - 9/5) = \frac{1}{125} (s_1(58 - 120s_2) - 9/5) < 0.
\]

The above observations imply that

\[
\frac{6}{5} = 1.2 < x_3 < 2.
\]

Moreover, since the average of the Laplacian eigenvalues of \( T \) satisfies \( 1 < \bar{\lambda} = 2 - 2/n < 2 \), we have \( \sigma \in \{2, 3\} \). We first observe that
\[ S_2(T) = x_1 + x_2 = n + 3 - x_3 - x_4 \]
\[ < n + 3 - \frac{1}{n} - 1.2 = n + 2 - \frac{1}{n} - \frac{1}{5} \]
\[ \leq |E| + 4 - \frac{2 \cdot 2 - 2}{n}. \]

Similarly, we have
\[ S_3(T) = x_1 + x_2 + x_3 = n + 3 - x_4 \]
\[ < n + 3 - \frac{1}{n} = n - 1 + (2 \cdot 3 - 1) - \left(1 + \frac{1}{n}\right) \]
\[ < |E| + (2 \cdot 3 - 1) - \frac{2 \cdot 3 - 2}{n}, \]

since \( n \geq 5 \). The fact that the inequality (2) holds for every \( k \) (and that it is never tight) is now a direct consequence of Lemma 3.1.

To conclude the proof, let \( T \) be a double broom with diameter 5, and assume that the number of leaves at each end are \( s_1, s_2 \geq 1 \), respectively. We first determine the value of \( \sigma \) using Algorithm Diagonalize. Indeed, using this algorithm for both \( \alpha = -1 \) and \( \alpha = -2 \), we conclude that there are three Laplacian eigenvalues larger than 1, which are also larger than 2. Now, since \( 1 < d < 2 \), we have \( \sigma = 3 \).

The characteristic polynomial of the Laplacian matrix associated with \( T \) is given by
\[ p(x) = q(x) \cdot (x - 1)^{n-5} \cdot x, \quad \text{where} \]
\[ q(x) = x^4 - (n + 3)x^3 + (s_1s_2 + 5n - 4)x^2 - (3s_1s_2 + 6n - 10)x + n. \]

It is clear that the three largest Laplacian eigenvalues of \( T \) are the three largest roots \( x_1, x_2, x_3 \) of \( q(x) \), and that the fourth root of \( q(x) \) is positive. Hence
\[ S_3(T) = x_1 + x_2 + x_3 \]
\[ = n + 3 - x_4 < n + 3 \]
\[ = |E| + 2 \cdot 3 - 1 - 1 \]
\[ < |E| + 2 \cdot 3 - 1 - \frac{4}{n}, \]

as \( n \geq 6 \). Once again, the fact that the inequality (2) holds for every \( k \) (and that it is never tight) follows directly from Lemma 3.1. \( \square \)

4. Star–NonStar trees

In this section, we consider the family \( \mathcal{F} \) of all trees \( T \) such that the deletion of any edge \( e \) of \( T \) whose endpoints are not leaves splits it into a star and a tree that is not a star. Because of this, we shall refer to the trees in this family as Star–NonStar trees (or SNS-trees for short). It is easy to see that one can view a tree in this family as a tree with a root vertex \( v_0 \) with which three different types of branches may be incident:

(i) a single vertex, also called pendant vertex, which we call a branch of type 0;
(ii) a tree of height one, called a branch of type 1;
(iii) a tree of height two whose root has degree one, called a branch of type 2.

Moreover, the trees in this family satisfy two additional properties: the combined number of branches of type 1 and 2 in a tree in \( \mathcal{F} \) is at least two (otherwise it has diameter three or it is a double broom with diameter four); when there are exactly two branches of type 1 and 2 incident with \( v_0 \) and at least
one of them has type 1, then \( v_0 \) is adjacent to pendant vertices (otherwise it is a double broom whose diameter is four or five).

It follows immediately from the definition that every tree in \( \mathcal{F} \) has one of three possible diameters: the absence of branches of type 2 implies diameter four; exactly one branch of type 2 leads to diameter five; two or more branches of type 2 give diameter six. Based on this, we say that a tree in \( \mathcal{F} \) lies in \( \mathcal{F}_4, \mathcal{F}_5 \) or \( \mathcal{F}_6 \) according to its diameter.

Henceforth, when referring to an SNS-tree \( T \), we use the following notation, which is depicted in Fig. 7. The tree \( T \) has a central node \( v_0 \), which is adjacent to three types of branches: \( p \geq 0 \) pendant vertices; \( r_1 \geq 0 \) branches of type 1, which are rooted at vertices \( v_1, \ldots, v_{r_1} \), where the branch rooted at \( v_i \) has \( s_i \geq 1 \) leaves; and \( r_2 \geq 0 \) branches of type 2, such that the \( j \)th branch of length 3 is rooted at a vertex \( w^*_j \), whose single neighbor \( w_j \) in the branch is adjacent to \( t_j \geq 1 \) leaves. Clearly, the total number vertices of a particular tree is \( n = p + r_1 + 2r_2 + 1 + \sum_{i=1}^{r_1} s_i + \sum_{j=1}^{r_2} t_j \), and, as mentioned above, a tree in this family can have diameter 4, 5 or 6. Additionally, we have \( r_1 + r_2 \geq 2 \), and, if \( r_1 + r_2 = 2 \) with \( r_1 \geq 1 \), we must have \( p \geq 1 \).

The three types of branches under consideration are special instances of generalized Bethe trees, which are rooted trees such that vertices at the same distance from the root have equal degrees. Rojo [11] has characterized the Laplacian spectrum of generalized Bethe trees whose roots are adjacent to a common root. Since the branches of an SNS-tree are all connected to a common root \( v_0 \), his result applies directly to our framework.

Let \( T \) be an SNS-tree. Adapting the notation from [11], we define, for \( i = 1, 2, \ldots, r_1 \), the matrix \( T_i \) of order 2 associated with the \( i \)th branch of type 1:

\[
T_i = \begin{pmatrix}
1 & \sqrt{s_i} \\
\sqrt{s_i} & s_i + 1
\end{pmatrix}.
\]

Moreover, for \( j = 1, 2, \ldots, r_2 \), we define the matrix \( Q_j \) of order 3 associated with the \( j \)th branch of type 2:

\[
Q_j = \begin{pmatrix}
1 & \sqrt{t_j} & 0 \\
\sqrt{t_j} & t_j + 1 & 1 \\
0 & 1 & 2
\end{pmatrix}.
\]
Given an SNS-tree $T$, let $M$ be the matrix defined as one of the matrices $M_p$ or $M_p^*$ below, according to whether $T$ has pendant vertices (matrix $M_p$) or not (matrix $M_p^*$):

$$
M_p = \begin{pmatrix}
1 & \sqrt{p} \\
T_1 & u_1 \\
\vdots & \vdots \\
T_{r_1} & u_{r_1} \\
Q_1 & \bar{u}_1 \\
\vdots & \vdots \\
Q_{r_2} & \bar{u}_{r_2} \\
\sqrt{p} \ u_1^T \ldots \ u_{r_1}^T \ \bar{u}_1^T \ldots \ \bar{u}_{r_2}^T & \delta
\end{pmatrix}
$$

(7)

$$
M_p^* = \begin{pmatrix}
T_1 & u_1 \\
\vdots & \vdots \\
T_{r_1} & u_{r_1} \\
Q_1 & \bar{u}_1 \\
\vdots & \vdots \\
Q_{r_2} & \bar{u}_{r_2} \\
\sqrt{p} \ u_1^T \ldots \ u_{r_1}^T \ \bar{u}_1^T \ldots \ \bar{u}_{r_2}^T & \delta
\end{pmatrix}
$$

(8)

Here $T_i, i = 1, \ldots, r_1$, and $Q_j, j = 1, \ldots, r_2$, are defined by Eqs. (5) and (6), respectively, $u_i = [0, 1]^T$, $\bar{u}_j = [0, 0, 1]^T$, and $\delta = r_1 + r_2 + p$ is the degree of $v_0$ in $T$.

The following result, which explicits the connection between the Laplacian spectrum of $T$ and the spectrum of the matrix $M$, can be read from Theorem 2 in [11].

**Lemma 4.1** (Rojo [11]). Let $T$ be an SNS-tree. The Laplacian spectrum of $T$ is the multiset given by the union of the spectrum of the matrix $M$ defined in Eq. (7) or (8) and of a multiset where all the elements are equal to 1.

One of the implications of this result is that all the Laplacian eigenvalues that are larger than their average $\bar{d}$ are also eigenvalues of the matrix $M$. Hence, in order to estimate the sum of the largest eigenvalues of $T$, we shall consider decompositions of $M$ into sums of matrices, to which we shall apply Theorem 2.1. If the SNS-tree $T$ contains $p \geq 1$ pendant vertices (hence $M = M_p$), we let

$$
M_p = \begin{pmatrix}
1 & \sqrt{p} \\
T_1 & u_1 \\
\vdots & \vdots \\
T_{r_1} & u_{r_1} \\
Q_1 & \bar{u}_1 \\
\vdots & \vdots \\
Q_{r_2} & \bar{u}_{r_2} \\
\sqrt{p} \ u_1^T \ldots \ u_{r_1}^T \ \bar{u}_1^T \ldots \ \bar{u}_{r_2}^T & \delta
\end{pmatrix} := A_p + B_p
$$
\[
\begin{pmatrix}
1 \\
T_1 \\
\vdots \\
T_{r_1} \\
Q_1 \\
\vdots \\
Q_{r_2} \\
\delta
\end{pmatrix}
\] + \[
\begin{pmatrix}
1 \\
\sqrt{p} u_1 \\
\vdots \\
\sqrt{p} u_{r_1} \\
\sqrt{p} u_{r_1}^T \\
\vdots \\
\sqrt{p} u_{r_2}^T \\
\delta
\end{pmatrix}
\] = \[
\begin{pmatrix}
1 \\
\sqrt{p} u_1 \\
\vdots \\
\sqrt{p} u_{r_1} \\
\sqrt{p} u_{r_1}^T \\
\vdots \\
\sqrt{p} u_{r_2}^T \\
\delta
\end{pmatrix}
\] \[= A_p + B_p = \]

Now, in the absence of pendant vertices in \( T \) (hence \( M = M_p \)), we let

\[
M_p = \begin{pmatrix}
T_1 & u_1 \\
\vdots & \vdots \\
T_{r_1} & u_{r_1} \\
Q_1 & \bar{u}_1 \\
\vdots & \vdots \\
Q_{r_2} & \bar{u}_{r_2} \\
\delta
\end{pmatrix}
\] := \[= A_p + B_p \]

Our next step is to apply Theorem 2.1 to the above decompositions of \( M \). To this end, we shall need the spectra of the matrices \( A \) and \( B \) (which have subindices “\( p \)” or “\( \overline{p} \)” according to whether \( M \) is equal to \( M_p \) or \( M_{\overline{p}} \)). With regard to the spectrum of \( B \), we rely on the following result.

**Lemma 4.2.** Let \( B \) be a symmetric matrix of order \( n \) for which all entries are zero, but for the last row and column, which are given by the vector \( (\sqrt{a_1}, \sqrt{a_2}, \ldots, \sqrt{a_{n-1}}, 0) \), where \( a_i \geq 0 \). The spectrum of \( B \) is given by \( \{\sqrt{\delta}, 0, 0, \ldots, 0, -\sqrt{\delta}\} \), where \( \delta = \sum_{i=1}^{n-1} a_i \).

**Proof.** Consider the matrix \( \lambda I - B \), whose determinant is the characteristic polynomial of \( B \). To put this matrix into upper triangular form, it suffices to replace the last row \( L_n \) by the linear combination \( L_n = \sum_{i=1}^{n-1} \frac{\sqrt{a_i}}{\lambda} L_i \), which does not affect the determinant. The resulting matrix has zeros below the diagonal, and its diagonal has \( n - 1 \) entries equal to \( \lambda \) and one entry equal to \( \lambda - \frac{\delta}{\lambda} \). Hence the characteristic polynomial of \( B \) satisfies \( p_B(\lambda) = \lambda^{n-2}(\lambda^2 - \delta) \), whose roots are precisely the elements in the statement of the lemma. \( \square \)
This result allows us to relate the largest Laplacian eigenvalues of $M$ with the largest eigenvalues of $A$ in the decompositions (9) and (10).

**Lemma 4.3.** Let $T$ be an n-vertex SNS-tree with Laplacian eigenvalues $\mu_1 \geq \cdots \geq \mu_n$, where exactly $\sigma$ of them are larger than their average $d$. Let $M = A + B$ be the matrix decomposition in (9) or (10) associated with it. Then, for $1 \leq k \leq \sigma$, it holds that

$$S_k(T) = \sum_{i=1}^{k} \mu_i \leq S_{k+1}(A) = \sum_{i=1}^{k+1} \lambda_i(A). \quad (11)$$

**Proof.** By applying Theorem 2.1 to $A + B$ with index set $I = \{1, \ldots, k, |M|\}$, where $|M|$ denotes the order of $M$, we obtain

$$\sum_{i \in I} \lambda_i(M) \leq \sum_{i=1}^{k} \lambda_i(A) + \sum_{i \in I} \lambda_i(B). \quad (12)$$

On the one hand, since $k \leq \sigma$, Lemma 4.1 tells us that the $k$ largest eigenvalues of $M$ correspond to the $k$ largest Laplacian eigenvalues of $T$. Moreover, we know that $\lambda_{|M|}(M)$ is the smallest Laplacian eigenvalue of $T$, hence $\lambda_{|M|}(M) = 0$. This implies that

$$\sum_{i \in I} \lambda_i(M) = \sum_{i=1}^{k} \mu_i = S_k(T).$$

On the other hand, the matrices $B_p$ and $B_\pi$ given in (9) and (10), respectively, have both the shape described in Lemma 4.2. Indeed, the nonzero entries in the last row of $B_p$ are $\sqrt{p}$ and $r_1 + r_2$ occurrences of 1, where $r_1$ and $r_2$ denote the number of branches of types 1 and 2 in $T$, respectively. In $B_\pi$, the nonzero entries are the $r_1 + r_2$ entries equal to 1. Observe that in both cases, the squares of the entries in the last row sum to the degree $\delta$ of the root $v_0$ in $T$. Since $I$ contains both 1 and $|M|$, Lemma 4.2 tells us that

$$\sum_{i \in I} \lambda_i(B) = \sqrt{\delta} - \sqrt{\delta} = 0.$$

As a consequence, Eq. (12) may be rewritten as

$$S_k(T) \leq \sum_{i=1}^{k} \lambda_i(A) = S_{k+1}(A),$$

as required. $\square$

To conclude this section, we describe the spectrum of $A$, which may be read directly from the spectra of its submatrices $T_i$ and $Q_i$.

**Lemma 4.4.** For every integer $s \geq 1$, the matrix

$$T = \begin{pmatrix} 1 & \sqrt{s} \\ \sqrt{s} & s + 1 \end{pmatrix}$$

has eigenvalues $x_1 > x_2$ satisfying

$$2 < x_1 < 2 + s - \frac{1}{2 + s}, \quad (13)$$

$$0 < x_2 < 1. \quad (14)$$

**Proof.** The characteristic polynomial of $T$ is given by $p(x) = x^2 - (s + 2)x + 1$, whose zeros are $x_1 = \frac{2 + s + \sqrt{2s^2 + 4s}}{2}$ and $x_2 = \frac{2 + s - \sqrt{2s^2 + 4s}}{2}$. The lower bounds in (13) and (14) are obvious. For the upper bounds, observe that, for every $a \geq 2$, 

$$\frac{2 + s + \sqrt{2s^2 + 4s}}{2} < 2 + s - \frac{1}{2 + s},$$

$$\frac{2 + s - \sqrt{2s^2 + 4s}}{2} < 1.$$
The upper bound in (13) is just the substitution of $a = s + 2$ in the above. On the other hand, given that $p(0) = 1$ and $p(1) = -s$, there must be a root of $p(x)$ between 0 and 1, establishing (14). □

Lemma 4.5. For every integer $t \geq 1$, the eigenvalues $y_1 > y_2 \geq y_3$ of the matrix

$$Q = \begin{pmatrix}
1 & \sqrt{t} & 0 \\
\sqrt{t} & t + 1 & 1 \\
0 & 1 & 2
\end{pmatrix}$$

satisfy the following:

$$2 < y_1 < t + 2 + \frac{1}{4t}$$

$$1 < y_2 < 2$$

$$y_3 > \begin{cases}
0.19 & \text{for } t = 1 \\
\frac{1}{4t} & \text{for } t \geq 2
\end{cases}$$

$$y_1 + y_2 = t + 4 - y_3.$$

Proof. The characteristic polynomial of the matrix $Q$ is equal to

$$p(x) = x^3 - (t + 4)x^2 + (2t + 4)x - 1.$$ 

This immediately implies that $y_1 + y_2 + y_3 = t + 4$. Our aim now is to locate the roots of this polynomial. To this end, observe that

$$p(0) = -1,$$

$$(4t)^3 \cdot (1/4t) = -32t^3 + 60t^2 - 16t - 1 < 0, \text{ for } t \geq 2,$$

$$p(1) = t > 0,$$

$$p(2) = -1,$$

$$p \left( t + 2 + \frac{1}{4t} \right) = \frac{(4t^2 - 4t - 1)^2}{64t^3} > 0.$$

When $t \geq 2$, since we know that $\lim_{x \to \infty} p(x) = \infty$, these facts imply that the polynomial $p(x)$ must have three real roots satisfying

$$\frac{1}{4t} < y_3 < 1 < y_2 < 2 < y_1 < t + 2 + \frac{1}{4t}.$$ 

When $t = 1$, we observe that $p(0.19) < 0$ and use the same argument. □
5. Theorem 1.1 for SNS-trees

In this section, we shall prove Theorem 1.1 when \( T \) is an SNS-tree. This section is organized in three parts, according to the diameter of the SNS-trees under consideration.

The following standard result will be useful. It can be proved by basic calculus tools.

**Lemma 5.1.** If \( \sum_{i=1}^{r} a_i = c \) for \( a_i \geq 1 \), \( 1 \leq i \leq r \), then
\[
\sum_{i=1}^{r} \frac{1}{a_i + 2} \geq \frac{r^2}{c + 2r}.
\]

5.1. Diameter 4

We first consider the class of SNS-trees with diameter four, which are denoted by \( F_4 \). Recall that this means that all the branches incident with the root vertex have type 0 or 1, and that there are at least two branches of the latter type (actually, in the absence of pendant vertices, there are at least three such branches, otherwise the tree would be a double broom with diameter four, which is not an SNS-tree). In the remainder of this section, let \( T \) be an \( n \)-vertex tree in \( F_4 \) with root vertex \( v_0 \). Assume that \( v_0 \) is incident with \( r \geq 2 \) branches of type 1, where the \( i \)th branch has root vertex \( v_i \) and \( s_i \geq 1 \) leaves. Further suppose that \( v_0 \) is incident with \( p \) pendant vertices.

As before, let \( \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0 \) be the Laplacian eigenvalues of \( T \), and let \( d = \frac{1}{n} \sum_{i=1}^{n} \mu_i \) be their average number. Moreover, let \( \sigma = \sigma(T) \) denote the number of eigenvalues of \( T \) that are larger than \( d \). The main goal of this section is to establish the following, which, in light of Lemma 3.1, implies the validity of Theorem 1.1 for trees in \( F_4 \).

**Lemma 5.2.** Given a \( n \)-vertex tree \( T \) in \( F_4 \), we have
\[
S_{\sigma} = \sum_{i=1}^{\sigma} \mu_i(T) < n - 1 + 2\sigma - 1 - \frac{2\sigma - 2}{n}.
\]

In order to prove this result, we first determine the possible values of \( \sigma \).

**Proposition 5.3.** Let \( T = (V, E) \) be an \( n \)-vertex tree in \( F_4 \), and assume that the root vertex is incident with \( r \geq 2 \) branches of type 1. Then the number of eigenvalues of \( T \) that are larger than the average value is either \( r \) or \( r + 1 \).

**Proof.** We use Algorithm Diagonalize to calculate \( a(v) \) with \( \alpha = -\overline{d} \) for every vertex \( v \in V \). Recall that the number of eigenvalues larger than \( \overline{d} \) is precisely the number of vertices \( v \) for which \( a(v) > 0 \). Here, the value of \( a(v) \) will vary according to whether \( v \) is equal to a leaf \( u \), to the root \( v_i \) of the \( i \)th type 1 tree, or to the root \( v_0 \). Indeed, it is easy to obtain the following expressions:
\[
a(u) = 1 - \left( 2 - \frac{2}{n} \right) = -\frac{n - 2}{n} < 0,
\]
\[
a(v_i) = s_i + 1 - \left( 2 - \frac{2}{n} \right) - \frac{s_i}{a(u)} = 2s_i + \frac{2s_i}{n - 2} + \frac{2}{n} - 1 > 0. \tag{15}
\]

This implies that the number of vertices \( v \) with \( a(v) > 0 \) is at least \( r \) and at most \( r + 1 \). \( \square \)

Our next task is to identify the trees in \( F_4 \) for which the number \( \sigma \) of eigenvalues that are larger than the average is precisely \( \sigma = r \), and hence those for which \( \sigma = r + 1 \). In other words, we characterize the trees \( T \) such that \( a(v_0) < 0 \), where
\[
a(v_0) = r + p - \left( 2 - \frac{2}{n} \right) + p \frac{n}{n - 2} - \sum_{i=1}^{r} \frac{1}{a(v_i)}. \tag{16}
\]
Lemma 5.4. If $T$ is a tree in $F_4$ for which the root is incident with at least one branch of type 0, then $a(v_0) > 0$.

Proof. Assuming that $p \geq 1$, Eq. (16) gives
\[
a(v_0) = r + p - \left(2 - \frac{2}{n}\right) + p \frac{n}{n-2} - \sum_{i=1}^{r} \frac{1}{a(v_i)}
\geq r + 1 - \left(2 - \frac{2}{n}\right) + \frac{n}{n-2} - \sum_{i=1}^{r} \frac{1}{a(v_i)}
= r + \frac{2}{n} + \frac{2}{n-2} - \sum_{i=1}^{r} \frac{1}{a(v_i)}
= \frac{2}{n} + \frac{2}{n-2} + \sum_{i=1}^{r} \left(1 - \frac{1}{a(v_i)}\right),
\]
Now, by Eq. (15), we know that $a(v_i) \geq \frac{2}{n} + \frac{2}{n-2} + 1 > 1$. In particular, the term $1 - \frac{1}{a(v_i)}$ in the above equation is always positive, and our result follows. \(\square\)

Lemma 5.5. If $T$ is a tree in $F_4$ for which the root is incident with at least three branches of type 1 with two or more leaves, then $a(v_0) > 0$.

Proof. Let $T$ be a tree in $F_4$ that is adjacent to $r$ branches of type 1, and assume without loss of generality that the branches rooted at vertices $v_1, v_2$ and $v_3$ satisfy $s_1, s_2, s_3 \geq 2$. We already know the result to be true when $v_0$ is adjacent to pendant vertices, so assume that there are no such vertices adjacent to $v_0$. Recall that
\[
a(v_0) = \frac{1}{r} - 2 + \frac{2}{n} - \sum_{i=1}^{r} \frac{1}{a(v_i)},
\]
where
\[
a(v_i) = 2s_i + \frac{2s_i}{n-2} + \frac{2}{n} - 1 > 2s_i - 1.
\]
As a consequence,
\[
1 - \frac{1}{a(v_i)} > \frac{1}{2s_i - 1} = \begin{cases} 
0, & \text{if } s_i = 1 \\
\frac{2}{3}, & \text{if } s_i \geq 2.
\end{cases}
\]
In particular, Eq. (17) becomes
\[
a(v_0) = -2 + \frac{2}{n} + \sum_{i=1}^{r} \left(1 - \frac{1}{a(v_i)}\right)
\geq -2 + \frac{2}{n} + 3 \cdot \frac{2}{3} = \frac{2}{n} > 0,
\]
as required. \(\square\)

We are now ready to prove Lemma 5.2.

Proof of Lemma 5.2. Let $T$ be an $n$-vertex tree in $F_4$. We shall prove our result according to the number $\sigma$ of Laplacian eigenvalues larger than the average $\bar{d}$, which, by Proposition 5.3, we know to be equal to $r$ or $r + 1$. 

Case 1 ($\sigma = r + 1$): To deal with this case, we shall apply Lemma 4.3 to $T$ with $k = r + 1$. It implies that

$$S_{r+1}(T) \leq S_{r+2}(A),$$

where $A$ is the matrix defined in (9) or (10) according to whether $v_0$ is adjacent to pendant vertices (i.e., $A = M_p$) or not (i.e., $A = M_F$).

Now, by Lemma 4.4, we know that the $r + 1$ largest eigenvalues of $A_T$ are the degree $\delta$ of $v_0$ and the largest eigenvalues of $T_1, \ldots, T_r$. Finally, $\lambda_{r+2}(A_T)$ is the largest among all smallest eigenvalues of $T_1, \ldots, T_r$, which is smaller than 1. On the other hand, the $r + 2$ largest eigenvalues of $A_T$ are, in nonincreasing order, $\delta$, the largest eigenvalues of $T_1, \ldots, T_r$, and 1. As a consequence, we know that, in both cases, $S_{r+1}(T)$ satisfies

$$S_{r+1}(T) \leq \delta + \sum_{i=1}^{r} \left( \frac{s_i + 2 + \sqrt{s_i^2 + 4s_i}}{2} \right) + 1$$

$$< \delta + 1 + \sum_{i=1}^{r} \left( s_i + 2 - \frac{1}{s_i + 2} \right)$$

$$= \delta + 1 + 2r + \sum_{i=1}^{r} s_i - \sum_{i=1}^{r} \frac{1}{s_i + 2}$$

$$= n + 2r - \sum_{i=1}^{r} \frac{1}{s_i + 2}$$

$$\leq n - 1 + 2(r + 1) - 1 - \frac{r^2}{\sum_{i=1}^{r} s_i + 2r}$$

$$= n - 1 + 2(r + 1) - 1 - \frac{r^2}{n + r - p - 1}.$$  

For (18), we used Lemma 4.4, for (19) and (21), we used that $n = 1 + p + r + \sum_{i=1}^{r} s_i$, while (20) comes from Lemma 5.1. We shall obtain our result if we prove that

$$\frac{r^2}{n + r - p - 1} \geq \frac{2(r + 1) - 2}{n} = \frac{2r}{n},$$

which is equivalent to showing that

$$n^2 \geq 2r(n + r - p - 1)$$

$$\iff n(r - 2) \geq 2(r - p - 1).$$

When $p \geq 1$, this follows immediately from the fact that $n > 2$. Now, if $p = 0$, we already know that $r \geq 3$ for $T$ to lie in the family $\mathcal{F}_A$. Then the result follows from the fact that $n > 4 \geq \frac{2(r-1)}{r-2}$, which holds because every branch of type 1 contains at least two vertices.

Case 2 ($\sigma = r$): We now consider the case when $\sigma = r$. By Lemma 5.4, we know that the root vertex $v_0$ is not adjacent to pendant vertices, which implies that $r \geq 3$. Moreover, Lemma 5.5 ensures that the number of branches $T_i$ of type 1 such that $s_i \geq 2$ is at most two.

Without loss of generality, assume that $s_i = 1$ for every branch $T_i, i = 3, \ldots, r$. To avoid subindices and simplify the notation, we also put $s_1 = a \geq s_2 = b$. Calculating the characteristic polynomial $p(x)$ of the Laplacian matrix, we have

$$p(x) = q_{a,b,r}(x) \cdot (x^2 - 3x + 1)^{r-3} \cdot (x - 1)^{n-2r-1} \cdot x,$$
where
\[ q_{a,b,r}(x) = x^6 - \left( a + b + r + 7 \right)x^5 + \left( ab + ar + br + 5a + 5b + 6r + 19 \right)x^4 \\
- \left( abr + 3ab + 4ar + 4br + 9a + 9b + 14r + 24 \right)x^3 \\
+ \left( 2abr + 3ab + 5ar + 5br + 7a + 7b + 16r + 13 \right)x^2 \\
- \left( 2ab + 2ar + 2br + 3a + 3b + 9r + 1 \right)x + a + b + 2r - 1. \]

Note that \( \frac{1}{2} \left( 3 + \sqrt{5} \right) > 2 \) is a root of \( p(x) \) with multiplicity \( r - 3 \), hence, assuming that \( \sigma = r \), we need to identify the other three Laplacian eigenvalues that are larger than the average \( \bar{d} \), all of which must be roots of \( q_{a,b,r}(x) \). Let \( x_1 \geq \cdots \geq x_6 \) be the roots of \( q_{a,b,r}(x) \).

If we apply Algorithm Diagonalize with \( \alpha = -1 \), we discover that there are exactly \( r \) roots of \( p(x) \) that are smaller than 1, and, since we know \( r - 2 \) of them, the other two must come from \( q_{a,b,r}(x) \). These two roots \( x_5, x_6 \) must be larger than or equal to the algebraic connectivity of \( T \), which, as \( T \) has diameter four, is at least \( \frac{1}{n} \) by Lemma 2.2.

Moreover, we may calculate
\[ q_{a,b,r}(1) = ab(r - 1) > 0, \]
\[ q_{a,b,r} \left( \frac{4}{3} \right) > 0. \]

To verify the second inequality, one may consider the change of variables \( q_{a' + 1, b' + 1, r' + 2}(x) \), where \( a', b', r' \) are nonnegative and observe that all the terms in the expansion of \( q_{a' + 1, b' + 1, r' + 2}(4/3) \) (whose indeterminates \( a', b', r' \) assume positive values) are positive.

Since three of the roots of \( q_{a,b,r}(x) \) must be above \( \bar{d} > 4/3 \), we conclude that there cannot be more than one root of \( q_{a,b,r}(x) \) in the interval \( (1, 4/3) \), and, by the above inequalities, there must be no roots at all in this interval. Therefore we have
\[ x_5 \geq x_6 \geq \frac{1}{n}, \quad x_4 > \frac{4}{3}. \]

The sum of all the roots of \( q_{a,b,r}(x) \) is equal to \( a + b + r + 7 \), so that, if we add the \( r \) largest roots of \( p(x) \), we obtain
\[ S_r = x_1 + x_2 + x_3 + (r - 3) \left( \frac{3 + \sqrt{5}}{2} \right) \]
\[ = a + b + r + 7 - x_4 - x_5 - x_6 + 3(r - 3) - (r - 3) \left( \frac{3 - \sqrt{5}}{2} \right) \]
\[ < a + b + 2r - 2 + 2r - \frac{4}{3} - \frac{2}{n} - (r - 3) \left( \frac{3 - \sqrt{5}}{2} \right) \]
\[ = n - 1 + 2r - 1 - (r - 3) \left( \frac{3 - \sqrt{5}}{2} \right) - \frac{2}{n} - \frac{1}{3}. \]

To conclude the proof, we need to verify that \( (r - 3) \left( \frac{3 - \sqrt{5}}{2} \right) + \frac{1}{3} + \frac{2}{n} > \frac{2r - 4}{n} \), which is equivalent to showing that
\[ (r - 3) \left( \frac{3 - \sqrt{5}}{2} \right) + \frac{1}{3} > \frac{2r - 4}{n} \]
\[ \iff n > \frac{2r - 4}{(r - 3) \left( \frac{3 - \sqrt{5}}{2} \right) + \frac{1}{3}}. \]
Since the expression on the right-hand side of this inequality does not surpass 6 for \( r \geq 3 \), and \( n \geq 2r + 1 \geq 7 \), our result follows. \( \square \)

5.2. Diameter 5

We now consider the class of SNS-trees with diameter five, which are denoted by \( \mathcal{F}_5 \). Here, there is precisely one branch of type 2 incident with the root vertex \( v_0 \) and \( r_1 \geq 1 \) branches of type 1. As with diameter four, for \( 1 \leq i \leq r_1 \), the \( i \)th branch of type 1 is denoted by \( T_i \) and has root vertex \( v_i \) and \( s_i \geq 1 \) leaves. The branch \( Q_1 \) is rooted at \( w \), with central vertex \( w \) and \( t \) leaves. Further suppose that \( v_0 \) is incident with \( p \) pendant vertices.

**Proposition 5.6.** If \( T = (V, E) \) is an \( n \)-vertex tree in \( \mathcal{F}_5 \) such that the root vertex is adjacent to \( r_1 \) branches of type 1, then the number of Laplacian eigenvalues of \( T \) that are larger than the average value \( \bar{a} \) is either \( r + 1 \) or \( r + 2 \), where \( r = r_1 + 1 \).

**Proof.** The value of \( a(v) \) may be calculated through Algorithm Diagonalize for every vertex \( v \) in \( T \). In fact, if \( u \) denotes a leaf of \( T \), we obtain that

\[
a(u) = 1 - \left( 2 - \frac{2}{n} \right) = -\frac{n - 2}{n} < 0 \tag{22}
\]

\[
a(v_i) = s_i + 1 - \left( 2 - \frac{2}{n} \right) - \frac{s_i}{a(u)} = 2s_i - 1 + \frac{2s_i}{n - 2} + \frac{2}{n} > 0 \tag{23}
\]

\[
a(w) = 2t - 1 + \frac{2t}{n - 2} + \frac{2}{n} > 0. \tag{24}
\]

This already implies that the number \( \sigma \) of vertices for which \( a(v) > 0 \) satisfies \( r_1 + 1 = r \leq \sigma \leq r + 2 \). To conclude the proof, we show that \( a(w^*) \) and \( a(v_0) \) cannot be both negative. To this end, assume that \( a(w^*) < 0 \), and observe that

\[
a(w^*) = \frac{2}{n} - \frac{1}{a(w)} = \frac{2}{n} - \frac{n(n - 2)}{(2t - 1)n^2 - (2t - 4)n - 4}, \tag{25}
\]

\[
a(v_0) = r + p - \left( 2 - \frac{2}{n} \right) + p\frac{n}{n - 2} - \sum_{i=1}^{r_1} \frac{1}{a(v_i)} - \frac{1}{a(w^*)}.
\]

It is easy to see that, if we look at \( a(w^*) \) as a function \( h(n) \) with \( t \geq 1 \) fixed, its derivative \( h' \) is negative for every \( n \geq 7 \). In particular, we have

\[
\lim_{n \to \infty} h(n) = \frac{-1}{2t - 1} \leq a(w^*) < 0, \tag{26}
\]

hence

\[
a(v_0) = r + p - \left( 2 - \frac{2}{n} \right) + p\frac{n}{n - 2} - \sum_{i=1}^{r_1} \frac{1}{a(v_i)} - \frac{1}{a(w^*)} \\
\geq -1 + \frac{2}{n} + \sum_{i=1}^{r_1} \left( 1 - \frac{1}{a(v_i)} \right) - \frac{1}{a(w^*)} \\
\geq -1 + \frac{2}{n} + \sum_{i=1}^{r_1} \left( 1 - \frac{1}{a(v_i)} \right) + 2t - 1 \\
\geq 2t - 2,
\]

which is nonnegative for \( t \geq 1 \), as required. In the above calculation, we are using the fact that \( 1 - \frac{1}{a(v_i)} \) is nonnegative for every \( i \). \( \square \)
Lemma 5.7. Given an $n$-vertex tree $T$ in $\mathcal{F}_5$, we have

$$S_\sigma = \sum_{i=1}^\sigma \mu_i(T) < n - 1 + 2\sigma - 1 - \frac{2\sigma - 2}{n}.$$ 

Proof. The proof of this result will be divided in two main parts: first we consider the case where the number $r_1$ of branches of type 1 incident with $v_0$ satisfies $r_1 \geq 2$. We then look at the case when $r_1 = 1$.

Case 1 ($r_1 \geq 2$): Proposition 5.6 implies that, to establish our result, it suffices to show that the upper bound holds for $S_{r+1}$ and for $S_{r+2}$. For the former, we shall now apply Lemma 4.3 with index set $I = \{1, 2, \ldots, r + 1, |M|\}$, where $|M|$ denotes the order of $M$. We reach

$$S_{r+1}(T) \leq S_{r+2}(A),$$

where $A$ is the block diagonal matrix given in (9) or (10) (as before, $A$ is also a matrix $A_p$ or a matrix $A_p^T$ according to whether $M$ is equal to $M_p$ or $M_p^T$, but this will not affect the remaining calculations).

Now, the $r + 2$ largest eigenvalues of $A$ are $\delta$, the largest eigenvalues of the matrices $T_1, \ldots, T_{r-1}$ (which are given in Lemma 4.4), and the largest and second largest eigenvalues of $Q_1$ (see Lemma 4.5 for the upper bound $t + 4$ on their sum). With this, we have

$$S_{r+2}(A) < \delta + \sum_{i=1}^{r_1} \left( s_i + 2 - \frac{1}{s_i + 2} \right) + t + 4 - y_3$$

$$= \delta + 2r_1 + t + 4 - y_3 + \sum_{i=1}^{r_1} s_i - \sum_{i=1}^{r_1} \frac{1}{s_i + 2}. $$

If we use $n = 1 + p + \left( r_1 + \sum_{i=1}^{r_1} s_i \right) + t + 2 = r + p + 2 + t + \sum_{i=1}^{r_1} s_i$ and apply Lemma 5.1 to bound the last summation, we obtain

$$S_{r+2}(A) < n - 2 + 4 - y_3 + 2r_1 - \frac{(r - 1)^2}{n + r - p - 4 - t}$$

$$\leq n - 1 + 2(r + 1) - 1 - y_3 - \frac{(r - 1)^2}{n + r - 4 - t}. $$

To conclude the proof, we show that $y_3 + \frac{(r - 1)^2}{n + r - 4 - t} \geq \frac{2r}{n}$. For $r = r_1 + 1 \geq 4$, this holds because $y_3 > 0$ and $t \geq 1$, so that

$$\frac{(r - 1)^2}{n + r - 5} \geq \frac{2r}{n} \iff n(r^2 - 2r + 1) > 2r(n + r - 5)$$

$$\iff nr^2 - 4rn + n > 2r(r - 5)$$

$$\iff n \geq \frac{2r(r - 5)}{r^2 - 4r + 1} = 2 - \frac{2r + 2}{r^2 - 4r + 1}. $$

Since $2 \geq \frac{2r + 2}{r^2 - 4r + 1} < 2 < n$, our claim follows. If $r_1 = 2$, we need to prove that $y_3 + \frac{4}{n - 1 - r} \geq \frac{6}{n}$. To this end, we use the bounds on $y_3$ provided by Lemma 4.5. On the one hand, if $t = 1$, we have

$$\frac{2n - 6 - 6t}{n(n - 1 - r)} < 0.19 \text{ for every positive } n \geq 3, \text{ and the result holds. On the other hand, if } t \geq 2, \text{ we have } y_3 \geq 4/t, \text{ so that}$$
On the other hand, we know that at least three eigenvalues of
Let\( x \) denote the number of leaves on the branches of type 1
where\( A \) is the corresponding block diagonal matrix. Observe that the \(( r + 3)\)rd largest eigenvalue of \( A \) satisfies \( \lambda_{r+3}(A) \leq 1 \), since it is either equal to 1 (if there are pendant vertices), equal to the second largest eigenvalue of a matrix of the type described in Lemma 4.4 or equal to the smallest eigenvalue of a matrix of the type described in Lemma 4.5. Thus, using the bound for \( S_{r+2}(A) \) obtained for \( \sigma = r + 1 \), we have
\[
S_{r+3}(A) = S_{r+2}(A) + \lambda_{r+3}(A)
\]
\[
\leq n - 1 + 2(r + 1) - 1 - \frac{2r}{n} + 1
\]
\[
= n - 1 + 2(r + 2) - 1 - \frac{2r}{n} - 1
\]
\[
< n - 1 + 2(r + 2) - 1 - \frac{2r + 2}{n}.
\]

Case 2 \(( r_1 = 1)\): In this case, we have \( r = 2 \) and \( p \geq 1 \), otherwise the tree would not be in \( \mathcal{F}_5 \). As the approach of the previous case fails here, we shall calculate the characteristic polynomial \( p(x) \) of the Laplacian matrix of \( T \) directly. Let \( s \) and \( t \) denote the number of leaves on the branches of type 1 and 2, respectively, so that \( n = 4 + p + s + t \). It can be seen that
\[
p(x) = q_{s,p,t}(x) \cdot (x - 1)^{n - 7} \cdot x
\]
\[
q_{p,s,t}(x) = x^5 - (t + s + p + 9)x^5 + (st + pt + ps + 7t + 7s + 6p + 31)x^4
\]
\[
- (pst + 5st + 4pt + 4ps + 17t + 17s + 13p + 53)x^3
\]
\[
+ (2pst + 7st + 5pt + 4ps + 18t + 18s + 13p + 48)x^2
\]
\[
- (3st + 2pt + ps + 8t + 8s + 6p + 22)x + (t + s + p + 4).
\]
Let \( x_1 \geq \cdots \geq x_6 \) be the roots of \( q_{p,s,t}(x) \). Applying Algorithm Diagonalize to \( T \) for \( \alpha = -1 \), we verify that there are three eigenvalues smaller than 1, two of which are \( x_5 \) and \( x_6 \), and four eigenvalues larger than 1, which are the four remaining roots of \( q_{p,s,t}(x) \). By Lemma 2.2, since the diameter of \( T \) is equal to five, we have
\[
\frac{4}{5n} \leq x_5, x_6 < 1.
\]
On the other hand, we know that at least three eigenvalues of \( T \) are above the average \( \bar{d} = 2 - 2/n \geq 2 - 2/7 > 7/5 \), so that there is at most one root of \( q_{p,s,t} \) in the interval \((1, 7/5)\). Since \( q_{p,s,t}(1) = pst > 0 \) and \( q_{p,s,t}(7/5) > 0 \), there can be no such root and
\[
1.4 < x_4 < 2.
\]
Here, to verify that \( q_{p,s,t}(7/5) > 0 \), we use the change of variables \( q_{p',s',t'+1}(x) \) for \( p', s', t' \geq 0 \) and we show that the terms in the expansion \( q_{p'+1,s'+1,t'+1}(7/5) \) have positive coefficients.
Assuming that \( \sigma = r + 1 = 3 \), the three largest eigenvalues of \( T \) are precisely the three largest roots of \( q_{p,s,1}(x) \). We thus have

\[
S_3(T) = n + 5 - x_4 - x_5 - x_6
\]

\[
< n + 5 - \frac{8}{5n} - 1.4
\]

\[
= n + 4 - \frac{8}{5n} - 0.4
\]

\[
< n + 4 - \frac{8}{5n} - \frac{12}{5n}
\]

\[
= n + 4 - \frac{4}{n}
\]

as required. To justify (27), observe that

\[
\frac{12}{5n} > 0.4 \iff n > 6,
\]

which holds for the trees in this family.

Now, if we assume that \( \sigma = r + 2 = 4 \), we have

\[
S_4(T) = n + 5 - x_5 - x_6
\]

\[
< n + 5
\]

\[
= n - 1 + 8 - 1 - 1
\]

\[
< n - 1 + 8 - 1 - \frac{6}{n},
\]

(28)

where, for (28), we use \( n \geq 7 \). This concludes our proof. □

5.3. Diameter 6

To conclude this section and the proof of Theorem 1.1 for SNS-trees, we consider the class of SNS-trees \( \mathcal{F}_6 \) with diameter six, which is denoted by \( \mathcal{F}_6 \). Here, there are at least two branches of type 2 incident with the root vertex \( v_0 \) and \( r_1 \geq 0 \) branches of type 1. As with diameter four, the \( i \)th branch of type 1 is denoted by \( T_i \) and has root vertex \( v_i \) and \( s_i \geq 1 \) leaves. The \( j \)th branch of type 2 is denoted by \( Q_j \) and is rooted at \( w_j^* \), with central vertex \( w_j \) and \( t_j \) leaves. Further suppose that \( v_0 \) is incident with \( p \) pendant vertices.

Proposition 5.8. If \( T = (V,E) \) is an \( n \)-vertex tree in \( \mathcal{F}_6 \) such that the root vertex is adjacent to \( r_1 \) branches of type 1 and \( r_2 \) branches of type 2, then the number \( \sigma \) of Laplacian eigenvalues of \( T \) that are larger than the average value \( \bar{d} \) satisfies \( r + 1 \leq \sigma \leq r + 4 \), where \( r = r_1 + r_2 \).

Proof. We apply Algorithm Diagonalize to calculate \( a(v) \) with \( \alpha = -\bar{d} \). In Eqs. (22)–(24), we may find general expressions for \( a(u) \) (where \( u \) is a leaf of \( T \)), \( a(v_i) \) (where \( v_i \) is the root of a branch of type 1) and \( a(w_j^*) \) (where \( w_j \) is the central vertex of a branch of type 2). As the value of \( a(v) \) is negative for the leaves, but positive for every \( v_i \) and \( w_j^* \), we know that \( r_1 + r_2 = r \leq \sigma \), and that \( \sigma = r + \ell \) if and only if precisely \( \ell \) vertices \( v \) amongst the roots \( w_j^* \) of the branches of type 2 and the vertex \( v_0 \) have positive \( a(v) \).

To prove our result, we show that:

(i) if \( a(w_j^*) < 0 \) for every branch of type 2, then \( a(v_0) > 0 \), so that \( \sigma \geq r + 1 \);

(ii) \( a(w_j^*) > 0 \) is positive for at most three branches of type 2, so that \( \sigma \leq r + 3 + 1 = r + 4 \).
We start with (i). It follows from (26) that \(-\frac{1}{a(w_j^r)} \geq 2t_j - 1\), and we know that \(1 - \frac{1}{a(v_i)} \geq 0\) for every \(i\). As a consequence,

\[
a(v_0) = r + p - \left(2 - \frac{2}{n}\right) + p \cdot \frac{n}{n-2} - \sum_{i=1}^{r_1} \frac{1}{a(v_i)} - \sum_{j=1}^{r_2} \frac{1}{a(w_j^r)} \\
= 2p + \frac{2p}{n-2} + \frac{2}{n} + r_2 - 2 + \sum_{i=1}^{r_1} \left(1 - \frac{1}{a(v_i)}\right) - \sum_{j=1}^{r_2} \frac{1}{a(w_j^r)} \\
> 2p + \frac{2}{n} + r_2 - 2 + r_1 \cdot 0 + \sum_{j=1}^{r_2} (2t_j - 1) \\
= 2p + \frac{2}{n} - 2 + 2 \sum_{j=1}^{r_2} t_j > 0,
\]

as both \(r_2\) and \(t_j\) are positive integers. This establishes (i).

For (ii), observe that Eq. (25) implies that, given a branch of type 2 with \(t_j\) leaves, we have \(a(w_j^r) > 0\) only if \(2 > \frac{n(n-2)}{(2t_j-1)^2-1} n^4\), which, isolating \(t_j\) (note that the denominators are positive), yields

\[
t_j \geq \frac{n^2 - 8n + 8}{4n(n-1)} = \frac{(n-2)(n^2 + 2n - 4)}{4n(n-1)} \\
\geq \frac{(n-2)(n^2 + 2n - 4)}{4n^2} = \frac{n-2}{4} \left(1 + \frac{2}{n} - \frac{4}{n^2}\right).
\]

Since \(n \geq 6\), we know that \(2/n > 4/n^2\), so that \(t_j \geq (n-2)/4\) whenever \(a(w_j^r) > 0\). In particular, if there are four vertices \(w_j^r\) with \(a(w_j^r) > 0\), say \(w_1^r, \ldots, w_4^r\), then \(t_1 + \cdots + t_4 \geq n - 2\), which is a contradiction (as at least nine vertices of \(T\) are not leaves of a branch of type 2, namely \(v_0\) and the two non-leaf vertices of each of the four branches of type 2). We conclude that at most three vertices \(w_j^r\) satisfy \(a(w_j^r) > 0\), which proves (ii). \(\Box\)

**Lemma 5.9.** Given an \(n\)-vertex tree \(T\) in \(F_6\), we have

\[
S_\sigma = \sum_{i=1}^{\sigma} \mu_i(T) < n - 1 + 2\sigma - 1 - \frac{2\sigma - 2}{n}.
\]  

**Proof.** Let \(T\) be a tree in \(F_6\) where the root \(v_0\) is attached to \(r_1 \geq 0\) branches of type 1, \(r_2\) branches of type 2 and \(p\) pendant vertices. In light of Proposition 5.8, it suffices to establish (29) for \(S_k\) with \(k \in \{r + 1, \ldots, r + 4\}\), where \(r = r_1 + r_2\).

As in the proof of Lemma 5.7, we apply Lemma 4.3. To find an upper bound on \(S_{r+\ell}(T)\) with \(\ell \in \{1, \ldots, 4\}\), we use the index set \(I = \{1, 2, \ldots, r + 1, \ldots, r + \ell, |M|\}\), where \(|M|\) denotes the order of \(M\). This leads to an analog of relation (11), namely

\[
S_{r+\ell}(T) \leq S_{r+\ell+1}(A),
\]

where \(A\) is the block diagonal matrix (as before, \(A\) is also a matrix \(A_p\) or a matrix \(A_{T}\) according to whether \(M\) is equal to \(M_p\) or \(M_T\), but this will not affect the remaining calculations).

Because of Lemmas 4.4 and 4.5, we know that the \(r + 1\) largest eigenvalues of \(A\) are \(\delta\) and the largest eigenvalues of each of the matrices associated with the \(r\) are branches of type 1 and 2 in \(T\). The next largest eigenvalues of \(A\) are chosen amongst the second largest eigenvalues of matrices associated with branches of type 2 (which lie between 1 and 2), the number 1 (which is an eigenvalue of \(A\) if \(T\) has at least one pendant vertex) and the smallest eigenvalues of the matrices associated with all branches (which lie between 0 and 1).
For the $r_1$ largest eigenvalues in matrices associated with branches of type 1, we shall use the upper bound $s_i + 2 - \frac{1}{s_i + 2}$ (the $i$th branch of this type has $s_i$ leaves). Analogously, for the $r_2$ largest eigenvalues in matrices associated with branches of type 2, we shall use the upper bound $t_j + 2 + \frac{1}{4t_j}$ (the $j$th branch of this type has $t_j$ leaves).

Now, by Lemma 4.5 (the sum of the eigenvalues of $Q_2$ is $t_j + 4$), the addition of the second, or even the third largest eigenvalue associated with a branch of type 2 would increase the upper bound of the previous paragraph by at most $2 - \frac{1}{4t_j} \geq \frac{7}{4}$, as $t_j \geq 1$. On the other hand, the addition of an eigenvalue 1 or a smallest eigenvalue of a matrix associated with a branch of type 1 contributes with at most 1 in this upper bound (the contribution of an additional eigenvalue of the branch with type 1 to the upper bound is at most $\frac{1}{s_i + 2}$). In other words, for $\ell \leq r_2$, if we assume without loss of generality that the additional contribution comes from the branches $Q_{r_2-\ell+1}, \ldots, Q_{r_2}$, we have

$$S_{r+\ell}(T) \leq \delta + \sum_{i=1}^{r_1} \left( s_i + 2 - \frac{1}{s_i + 2} \right) + \sum_{j=1}^{r_2} \left( t_j + 2 + \frac{1}{4t_j} \right) + \sum_{j=1}^{r_2-\ell} \left( 2 - \frac{1}{4t_j} \right)$$

$$= \left( \delta + r_2 + \sum_{i=1}^{r_1} s_i + \sum_{j=1}^{r_2} t_j \right) + 2r_1 + r_2 + 2\ell + \sum_{j=1}^{r_2-\ell} \frac{1}{4t_j} - \sum_{i=1}^{r_1} \frac{1}{s_i + 2}$$

$$= n - 1 + (2r + \ell - 1) - r_2 + 2\ell + \sum_{i=1}^{r_1} \frac{1}{4t_j} - \sum_{i=1}^{r_1} \frac{1}{s_i + 2}$$

$$\leq n - 1 + (2r + \ell - 1) - r_2 + 2\ell - \frac{r_2 - \ell}{4} - \sum_{i=1}^{r_1} \frac{1}{s_i + 2}$$

$$= n - 1 + (2r + \ell - 1) - \left( \frac{3r_2}{4} + \frac{\ell}{4} - 1 + \sum_{i=1}^{r_1} \frac{1}{s_i + 2} \right).$$

Now, if $r_2 < \ell$, say $r_2 = \ell - \ell^*$, an upper bound is obtained when the contribution of $\ell^*$ of the additional eigenvalues is set to 1, from which one may easily derive

$$S_{r+\ell}(T) \leq n - 1 + (2r + \ell - 1) - \left( \ell - 1 + \sum_{i=1}^{r_1} \frac{1}{s_i + 2} \right).$$

However, note that

$$\ell = \frac{3}{4} \ell + \frac{\ell}{4} = \frac{3r_2}{4} + \frac{\ell}{4}.$$

Hence, to conclude our proof, it suffices to show that

$$\frac{3r_2}{4} + \frac{\ell}{4} - 1 + \sum_{i=1}^{r_1} \frac{1}{s_i + 2} > \frac{2(r + \ell) - 2}{n}. \quad (30)$$

We first assume that $\ell \geq 2$, in which case we are able to show the tighter bound

$$\frac{3r_2}{4} + \frac{\ell}{4} - 1 > \frac{2(r + \ell) - 2}{n},$$

which is equivalent to

$$n > \frac{8(r + \ell - 1)}{3r_2 + \ell - 4} = 8 \cdot \frac{3r_2 + \ell - 4 + r_1 - 2r_2 + 3}{3r_2 + \ell - 4}$$

$$= 8 \left( 1 + \frac{r_1 - 2r_2 + 3}{3r_2 + \ell - 4} \right).$$
Since \( T \) contains \( r_1 \) branches of type 1 (each of which has at least two vertices) and \( r_2 \geq 2 \) branches of type 2 (each of which contains at least three vertices), we know that \( n \geq 1 + 2r_1 + 3r_2 \). Since \( r_2 \geq 2 \), we have \( n \geq 7 + 2r_1 \) and

\[
\frac{r_1 - 2r_2 + 3}{3r_2 + \ell - 4} \leq \frac{r_1 - 1}{4}.
\]

In particular,

\[
8 \left( 1 + \frac{r_1 - 2r_2 + 3}{3r_2 + \ell - 4} \right) \leq 8 + \frac{8(r_1 - 1)}{4} = 6 + 2r_1,
\]

which is smaller than \( 7 + 2r_1 \leq n \), thus verifying Eq. (30).

Now, assume that \( \ell = 1 \). If \( r_1 = 0 \) (hence \( r_2 = r \)), Eq. (30) holds because

\[
3r - 3 > \frac{2r}{n}
\]

for every \( n \geq 7 \) and \( r \geq 2 \).

For \( r_1 \geq 1 \), let \( S = \max\{s_i : i = 1, \ldots, r_1\} \). To establish Eq. (30), we show that

\[
\frac{3r_2}{4} - \frac{3}{4} + \frac{r_1}{S + 2} > \frac{2r}{n},
\]

which may be rewritten as

\[
n > \frac{8r}{3r_2 - 3 + 4r_1/(S + 2)}.
\]

However, we know that \( n \geq 7 + S + (r_1 - 1)2 = 5 + 2r_1 + S \) and that

\[
\frac{8r_1 + 8r_2}{3r_2 - 3 + 4r_1/(S + 2)} = 8 \cdot \left( 1 + \frac{r_1 - 2r_2 + 3 - 4r_1/(S + 2)}{3r_2 - 3 + 4r_1/(S + 2)} \right) \leq 8 \cdot \left( 1 + \frac{r_1 - 1 - 4r_1/(S + 2)}{3 + 4r_1/(S + 2)} \right) = 5 + \frac{8r_1 + 1 - 20r_1/(S + 2)}{3 + 4r_1/(S + 2)}.
\]

Thus the result is true if we show that

\[
2r_1 + S > \frac{8r_1 + 1 - 20r_1/(S + 2)}{3 + 4r_1/(S + 2)},
\]

which holds if and only if

\[
(2r_1 + S)(3 + 4r_1/(S + 2)) > 8r_1 + 1 - 20r_1/(S + 2)
\]

\[
\iff r_1 ((4S + 20)/(S + 2) - 2) + 3S - 1 + 8r_2^2/(S + 2) > 0.
\]

The last assertion holds since both \((4S + 20)/(S + 2) - 2\) and \(3S - 1\) are positive. This concludes the proof. \( \Box \)

### 6. Proof of Theorem 1.1

We are now ready to prove Theorem 1.1 in general, which we now restate.

**Theorem 6.1.** Let \( T = (V, E) \) be a tree on \( n \) vertices with Laplacian eigenvalues \( \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0 \). Then, for every \( k \in \{1, \ldots, n\} \) it holds that
\[ S_k(T) \leq \sum_{i=1}^{k} \mu_i = |E| + 2k - 1 - \frac{2k - 2}{n} = n + 2k - 2 - \frac{2k - 2}{n}. \]

Moreover, equality is achieved only when \( k = 1 \) and \( T \) is a star on \( n \) vertices.

**Proof.** The proof is by induction on the number of vertices. When \( n \leq 3 \), every tree \( T \) on \( n \) vertices is a star and the result is true by Lemma 3.2.

Let \( T = (V, E) \) be a tree on \( n \geq 4 \) vertices and assume that the result holds for every tree with fewer vertices. We prove that the inequality in the statement of the theorem holds strictly. Since \( T \) is not a star, it has diameter at least three. In particular, \( T \) contains an edge \( e \) whose endpoints are not leaves. Moreover, since we know the bound to be true for \( S\&S \)-trees and \( SNS \)-trees, we may suppose that there exists such an edge \( e \) with the additional property that the forest \( F = T \setminus \{e\} \) is the union of two trees \( T_1 = (V_1, E_1) \) and \( T_2 = (V_2, E_2) \), none of which is a star. Let \( n_1 \) and \( n_2 \) denote the number of vertices in each tree, respectively, so that \( n_1 + n_2 = n \). Let \( M_T \) and \( M_F \) denote the Laplacian matrices of \( T \) and \( F \), respectively, for which the two endpoints of \( e \) correspond to the first two rows. Clearly, we have \( M_T = M_F + M' \), where

\[
M' = \begin{pmatrix}
0 & \cdots & 0 \\
A & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 
\end{pmatrix},
\]

with

\[
A = \begin{pmatrix}
1 & -1 \\
-1 & 1 
\end{pmatrix}.
\]

The characteristic polynomial of \( M' \) is \( p(x) = x^{n-1}(x - 2) \), and we obtain the inequality

\[ S_k(T) \leq S_k(F) + 2 \quad (31) \]

by applying Theorem 2.1 to the \( k \) largest eigenvalues of \( M_T \) with \( B = M' \) and \( C = M_F \). The set of the eigenvalues of \( M_F \) is the union of the sets of Laplacian eigenvalues of \( T_1 \) and \( T_2 \). Let \( k_1 \) and \( k_2 \) denote the number of Laplacian eigenvalues of \( T_1 \) and \( T_2 \) amongst the \( k \) largest Laplacian eigenvalues of \( T \), respectively, and assume without loss of generality that \( k_1 \geq k_2 \). Eq. (31) may be rewritten as

\[ S_k(T) \leq S_{k_1}(T_1) + S_{k_2}(T_2) + 2. \quad (32) \]

The case when \( k_2 \neq 1 \) is straightforward. Indeed, if \( k_2 = 0 \), all the large eigenvalues of \( T \) come from \( T_1 \). As a consequence, we may apply the induction hypothesis to \( T_1 \) (recall that \( |E_1| \leq |E| - 2 \) and \( n_1 < n \)) in Eq. (32) to obtain

\[
S_k(T) \leq S_k(T_1) + 2 \\
\leq |E_1| + 2k - 1 - \frac{2k - 2}{n_1} + 2 \\
\leq |E| + 2k - 1 - \frac{2k - 2}{n_1} \\
< |E| + 2k - 1 - \frac{2k - 2}{n},
\]

as required.
Now, for $k_1 \geq k_2 \geq 2$, we use induction for both $T_1$ and $T_2$ in Eq. (32):

\[
S_k(T) \leq S_{k_1}(T_1) + S_{k_2}(T_2) + 2 \\
\leq |E_1| + 2k_1 - 1 - \frac{2k_1 - 2}{n_1} + |E_2| + 2k_2 - 1 - \frac{2k_2 - 2}{n_2} + 2 \\
= |E| + 2k - 1 - \frac{2k_1 - 2}{n_1} - \frac{2k_2 - 2}{n_2}.
\]

(33)

The desired conclusion will follow from the following auxiliary lemma.

**Lemma 6.2.** If $a$, $b$, $c$, $d$ are positive real numbers satisfying $ab > 1$, we have

\[
\frac{a}{c} + \frac{b}{d} > \frac{a + b + 2}{c + d}.
\]

**Proof.** In order to establish this result, it suffices to show that $(c + d)(ad + bc) > cd(a + b + 2)$, which is equivalent to $ad^2 + bc^2 > 2cd$. Now, because $ab > 1$, we have

\[
ad^2 + bc^2 - 2cd > ad^2 + bc^2 - 2\sqrt{abcd} = (\sqrt{ad} - \sqrt{bc})^2 \geq 0,
\]

as required. \(\square\)

To obtain our result from Eq. (33), we apply Lemma 6.2 with $a = 2k_1 - 2 \geq 2$, $b = 2k_2 - 2 \geq 2$, $c = n_1$ and $d = n_2$ to conclude that

\[
\frac{2k_1 - 2}{n_1} + \frac{2k_2 - 2}{n_2} > \frac{2(k_1 + k_2) - 2}{n_1 + n_2} = \frac{2k - 2}{n},
\]

again establishing the desired result.

Henceforth, we suppose that $k_2 = 1$. The remainder of the proof will be organized in two parts, according to the value of $k_1$.

First suppose that $k_1 = 1$. Since $T_2$ is not a star, we know that $n_2 \geq 4$, hence $n \geq 6$, and that Lemma 2.3 may be applied to $T_2$. If we apply the induction hypothesis to $T_1$, we obtain

\[
S_2(T) \leq S_1(T_1) + S_1(T_2) + 2 \\
\leq n_1 + n_2 - \frac{1}{2} + 2 \\
= |E| + 4 - 1 - \frac{1}{2} \\
< |E| + 2 \cdot 2 - 1 - \frac{2}{n},
\]

as required.

Now, assume that $k_1 \geq 2$. Again from the fact that $T_2$ is not a star, we know that the second largest degree in its degree sequence satisfies $d_2(T_2) \geq 2$. By the result below, due to Brouwer and Haemers [1], it holds that the second largest Laplacian eigenvalue of $T_2$ satisfies $\mu_2(T_2) \geq d_2(T_2) - 2 + 2 \geq 2$.

**Lemma 6.3.** Let $G$ be a connected graph with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$ and Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. Then we have

\[
\mu_i \geq d_i - i + 2.
\]

Now, using the fact that $\mu_2(T_1) \geq \mu_2(T_2) \geq 2$, we deduce that $T_1$ is not a star, hence $n_1 \geq 4$. We combine the induction hypothesis for $T_1$ and Lemma 2.3 for $T_2$ to obtain
\[ S_k(T) \leq S_{k-1}(T_1) + S_1(T_2) + 2 \]
\[ \leq |E_1| + 2(k - 1) - 1 - \frac{2k - 4}{n_1} + n_2 - \frac{1}{2} + 2 \]
\[ = n_1 - 1 + n_2 + 2k - 1 - \frac{2k - 4}{n_1} - \frac{1}{2} \]
\[ = |E| + 2k - 1 - \frac{2k - 2}{n_1} - \frac{n_1 - 4}{2n_1} \]
\[ \leq |E| + 2k - 1 - \frac{2k - 2}{n_1} \]
\[ < |E| + 2k - 1 - \frac{2k - 2}{n}, \]
concluding our proof. Observe the use of the inequality \( n_1 \geq 4 \) when going from the fourth to the fifth line in the above equation. \( \square \)

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References