Automated conjectures on upper bounds for the largest Laplacian eigenvalue of graphs

V. Brankov\textsuperscript{a}, P. Hansen\textsuperscript{b}, D. Stevanović\textsuperscript{c}

\textsuperscript{a}Mathematical Institute, Serbian Academy of Science and Arts, Knez Mihajlova 35, 11000 Belgrade, Serbia and Montenegro

\textsuperscript{b}GERAD, HEC, 3000 Chemin de la Côte-Sainte-Catherine, Montréal H3T 2A7, Canada

\textsuperscript{c}Faculty of Science and Mathematics, Višegradska 33, 18000 Niš, Serbia and Montenegro

Abstract

Several upper bounds on the largest Laplacian eigenvalue of a graph $G$, in terms of degree and average degree of neighbors of its vertices, have been proposed in the literature. We show that all these bounds, as well as many conjectured new ones, can be generated systematically using some simple algebraic manipulations. Bounds depending on the edges of $G$ are also generated. Moreover, the interestingness of bounds is discussed, in terms of dominance and tightness. Finally, we give a unified way of proving a sample of these bounds.

Keywords: Conjecture; Automatic generation of conjectures; Laplacian matrix; Laplacian eigenvalues; Graph.

AMS Classification: 05C50

1 Introduction

Graph theory is replete with lower and upper bounds on the value of an invariant of a graph $G$ in terms of one or several other ones. Often, several bounds involve the same invariant. There may even be many bounds for which this is so. A typical such case is that of upper bounds for the largest eigenvalue $\mu$ of the Laplacian matrix of a graph $G$. This eigenvalue has found numerous applications so far: for example, it is used in theoretical chemistry, within the Heilbronner model, to determine the first ionization potential of alkanes (see [20]), in combinatorial optimization to provide an upper bound on the size of the maximum cut in graph (see [31, 11, 12, 13] and [32, Sections 3.1 and 7.3]), in communication networks to provide a lower bound on the edge-forwarding

\textsuperscript{1}The first and the third authors acknowledge support by Grant 1389 of Serbian Ministry of Science. This paper was written in part during a visit of the first author and two visits of the third author to GERAD, Montréal. Support of GERAD and the Data Mining Chair of HEC Montréal is gratefully acknowledged. The second author was supported by NSERC grant #105574–02.
For more information on the applications of this and other Laplacian eigenvalues of a graph, see a comprehensive survey [30].

Recall that the adjacency matrix $A = (a_{ij})$ of a graph $G = (V, E)$ with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set $E$ is such that $a_{ij} = 1$ if vertices $v_i$ and $v_j$ are adjacent (joined by an edge, i.e., $\{v_i, v_j\} \in E$, which we also denote by $v_i \sim v_j$) and $a_{ij} = 0$ otherwise. The Laplacian matrix $L = D - A$ of $G$ is the difference of a diagonal matrix $D = (d_i)$, with $d_i = \sum_{j=1}^{n} a_{ij}$ equal to the degree of $v_i$ for $i = 1, 2, \ldots, n$, and of matrix $A$.

A number of upper bounds on the largest eigenvalue $\mu$ of the Laplacian matrix $L$ have been proposed in the literature. Let $m_i$ denote the average of the degrees of the neighbors of vertex $v_i$:

$$m_i = \frac{1}{d_i} \sum_{j=1}^{n} a_{ij} d_j, \quad i = 1, 2, \ldots, n.$$  \hspace{1cm} (1)

Several of these bounds are of the form

$$\mu \leq \max_{v_i} f(d_i, m_i);$$  \hspace{1cm} (2)
The concept of interestingness of a mathematical result is a difficult one to make precise (see e.g. [7] and [21, 23]); hence we will limit ourselves to express it in the form of dominance (i.e., for a given set of graphs, is a bound never smaller than another one, or never smaller than the best of several other ones) tightness (i.e., for a given set of graphs, how often is the bound satisfied as an equality), and precedence (i.e., for a given set of graphs, how often does the bound yield the best value among a given set of bounds). This discussion will lead us to a tentative answer as to which bounds among many are worthy of being retained.

The paper is organized as follows: previous work on automated and computer-aided generation of conjectures, as well as selection among conjectures, is summarized in the next section. Elementary transformations leading to upper bounds of the forms (2) and (3) and a selection of bounds are discussed in Section 3. Some typical bounds are proved to be valid in Section 4 (proving them all would be very long and tedious, if not impossible). Brief conclusions are drawn in Section 5. Lists of conjectured bounds obtained and known ones reproduced are given in the appendices.

2 Previous work on automated and computer-aided generation and selection of conjectures

Computers play an increasing and increasingly distinguished role in graph theory, see e.g. [22] for a survey. In particular, several systems help to obtain conjectures in a computer-aided or automated way:

(i) the system GRAPH of Cvetković and coauthors [8, 9], developed in the early eighties, allows interactive representation and modification of a graph G, as well as various operations on it, and computation of many invariants. It thus greatly enhances the formulation of conjectures, in a process similar to the usual pencil-and-paper one of the graph theorist;

(ii) the system INGRID of Brigham et al. [14, 15, 16] gathers in a database relations on several graph invariants, which can be put into the form of bounds and used for various purposes;

(iii) the system GRAFFITI of Fajtlowicz [17, 18] generates a priori, in early versions, conjectures of the form $i_1(G) \leq i_2(G)$, $i_1(G) \leq i_2(G) + i_3(G)$, or $i_1(G) \cdot i_2(G) \leq i_3(G)$ where $i_1(G)$, $i_2(G)$ and $i_3(G)$ are invariants or small integers, and in more recent versions, also expressions involving in addition to the four operations $+, -, \cdot, /$, the exponent, logarithm, floor and ceiling, etc. The user decides which invariants to consider and, possibly, which operations to apply but apparently not in which order they are applied (details on the way nonlinear relations are obtained are not given);

(iv) the AutoGraphiX system of Caporossi and Hansen [3, 4] generates a parametric family of optimal or near-optimal graphs for a given invariant (or for a formula involving several invariants, which may itself be viewed as an
invariant) using the Variable Neighborhood Search metaheuristic [24, 29].

The conjectures are obtained in one (or more) of the three following ways:

(iv.a) a numerical approach which uses the mathematics of principal component analysis to find a basis of affine relations between the invariants considered, satisfied by these graphs;

(iv.b) a geometric approach which considers the graphs obtained as points in invariant space and applies a “gift-wrapping” algorithm to determine the convex hull. Each facet of this convex hull corresponds to a linear inequality between graph invariants (the recent system GraPHedron, developed by Mélot et al. [5], follows a similar approach but replacing determination of optimal or near-optimal graphs by enumeration of all graphs with a small number of vertices);

(iv.c) an algebraic approach which recognizes the classes to which the graphs obtained belong, then uses a database of relations giving expressions of the invariants considered on these classes in function of the order of the graphs; these formulas are then substituted for the invariants and simplified;

(v) the HR (for Hardy and Ramanujan) system of Colton [7] generates relations of the form

$$t_1(G) + t_2(G) \leq c,$$

where $t_1(G)$ and $t_2(G)$ are terms composed of an invariant or the product of two invariants possibly with a minus sign and $c$ is a small integer usually 0, 1 or 2, again possibly with a minus sign.

The conjecture generating procedures that we present in this paper are more specific than those described above in that they apply to bounds for a precise invariant of a given form (i.e., (2) and (3)). As will be seen they are also more general in the type of relation obtained and yield a large number of them.

Conjectures are clearly of variable interest, a concept which may be understood as having many dimensions; in addition to correctness, which is uncontroversial, one may consider surprisingness, simplicity, non-dominance, tightness (or sharpness), and so forth.

We focus on dominance and tightness used in some of the above systems:

(i) INGRID [16] examines whether a relation is a consequence of others, for families of graphs specified by choosing intervals of value for the invariants involved. Then these bounds are refined by applying relations from the database. If one interval becomes empty, this indicates a contradiction. Such a scheme can be used to show that no graph in the set considered gives a larger value to the bound studied than the conjunction of all others. It is then conjectured that this is true in general, which may be proved or disproved by hand. If it is true, the bound need not be added to (or may be deleted from) the database.

(ii) the DALMATIAN version of GRAFFITI [18] uses the same approach except that the graphs considered are those given in a small database (where
values of invariants are stored) containing a few hundred of them and checking is done by direct computation. A bound is viewed as informative if it gives a better value than the conjunction of all others in the database.

(iii) in its most recent version [2], AutoGraphiX eliminates many simple conjectures by proving them automatically in various ways; they are then viewed as observations and the remaining, usually more difficult, ones are proved by hand, if possible. Recently, a large proportion of a set of several hundred conjectures of HR were also proved automatically by AutoGraphiX, a few of them were disproved by that system or by specific counterexamples; all but one of those remaining could be proved by hand.

3 Automatic generation of conjectured bounds

The set of conjectured upper bounds on \( \mu \) is obtained in several steps. In the first step we generate a number of candidate bounds using a few simple algebraic transformations. In the second step we test them on a number of connected graphs and refute those for which there exists a counterexample. Then, in the third step we check the dominance among bounds and retain only those that are not dominated by another bound. Finally, we provide a few simple statistics on the remaining bounds to gain some insight into which of them are, in a sense, the most important ones.

3.1 Step 1: Generating

We first describe elementary transformations leading to expressions of the upper bounds in forms (2) and (3). The starting point is a simple observation that all examples of bounds on page 2 attain equality in the case of bipartite regular graphs. Indeed, in such a case we have that \( d_v = m_v = x \) holds for each \( v \in V \) and \( \mu = 2x \). Thus, a natural condition for a function \( f \) in a conjectured bound

\[
\mu \leq \max_{v_i} f(d_i, m_i)
\]

is that it satisfies

\[
f(x, x) = 2x.
\] (4)

Similarly, for a function \( f \) in a conjectured bound

\[
\mu \leq \max_{v_i \sim v_j} f(d_i, m_i, d_j, m_j),
\]

a natural condition is that it satisfies

\[
f(x, x, x) = 2x.
\] (5)

Whenever the appropriate condition (4) or (5) is satisfied, the candidate bounds will be tight, i.e., it will attain equality for bipartite regular graphs.
We generate the bounds in such a way that the respective condition (4) or (5) is always satisfied. For this reason, we first generate a set $\mathcal{B}_v$ of arithmetic expressions in one variable $x$. Initially, we set $\mathcal{B}_v = \{2x\}$. Supposing that $f, g \in \mathcal{B}_v$, we form a new expression according to one of the following transformations:

(tv1) $f' := \frac{f + g}{2}$;
(tv2) $cf' := kf + (c - k)g$, where $c \in \mathbb{N}$ and $1 \leq k < c$;
(tv3) $f' := \frac{xf}{x}$;
(tv4) $f' := \sqrt{f \cdot g}$.

It is easy to prove by induction that all expressions in $\mathcal{B}_v$ evaluate to $2x$ after simplification. However, we do not simplify expressions from $\mathcal{B}_v$. The reason lies in the fact that, in order to get a bound of the form (2) from an expression $f \in \mathcal{B}_v$, we replace each occurrence of $x$ in $f$ with either $d_i$ or $m_i$. Thus, if $|f|$ is the number of occurrences of $x$ in $f$, we get $2^{|f|}$ conjectured bounds from an expression $f$. Only after this step we simplify the final expressions in $d_i$ and $m_i$.

For example, we can get the bound

$$\mu \leq \max_{v_i} d_i + \sqrt{d_i m_i} \quad [35]$$

in the following manner:

- start with the expression $2x$;
- apply (tv4) to get an expression $\sqrt{2x \cdot 2x}$;
- apply (tv1) to get an expression $\frac{2x + \sqrt{2x \cdot 2x}}{2}$;
- replace the first and the second occurrence of $x$ in the previous expression by $d_i$ and the last occurrence of $x$ by $m_i$, and then simplify to get an expression $d_i + \sqrt{d_i m_i}$.

The situation is slightly different for the bounds of the form (3). Namely, since edge ends are indistinguishable in simple graphs, the bounding functions $f(d_i, m_i, d_j, m_j)$ have to be symmetric with respect to $i$ and $j$. We first generate a set $\mathcal{B}_e$ of arithmetic expressions in one variable $x$. Initially, we set $\mathcal{B}_e = \{2x\}$. Supposing that $f, g \in \mathcal{B}_e$, we form a new expression according to one of the following transformations:

(te1) $f' := \frac{f + g}{2}$;
(te2) $cf' := kf + (c - k)g$, where $c \in \mathbb{N}$ and $1 \leq k < c$;
(te3) $f' := \frac{xf}{2x}$;
(te4) $f' := \sqrt{f \cdot g}$;
(te5) $f' := 2 + \sqrt{f \cdot f - 4f + 4}$.
(te6) $f'$ is obtained by replacing $cx^k$ in $f$ with $cx^k + 2x^k -2x^k$, $c \in \mathbb{N}$.

It is again easy to prove by induction that all expressions in $B_c$ evaluate to $2x$ after simplification. Next, in order to get a conjectured bound symmetric with respect to $i$ and $j$, we replace each occurrence of $x$ in an expression from $B_c$ in one of the following ways:

(re1) $cx^k$ is replaced by $cd_i^p m_i^q + cd_j^p m_j^q$, $p + q = k$, $p \geq 0$, $q \geq 0$;

(re2) $2cx^k$ is replaced by $cd_i^p m_i^q + cd_j^p m_j^q$, $p + q = k$, $p \geq 0$, $q \geq 0$.

After this step, we simplify the final expressions in $d_i, d_j, m_i$ and $m_j$.

For example, we can get the conjectured bound

$$\mu \leq \max_{v_i \sim v_j} 2 \frac{d_i^2 + d_j^2}{m_i + m_j}$$

in the following manner:

- start with the expression $2x$;
- apply (te3) to get $\frac{2x^2}{2x}$;
- apply (re2) to $2x^2$ in the numerator with $p = 2$, $q = 0$, to get $d_i^2 + d_j^2$;
- apply (re2) to $2x$ in the denominator with $p = 0$, $q = 1$, to get $m_i + m_j$.

The transformations (tv1)–(tv4) and (te1)–(te6) are chosen to be as simple as possible, while being powerful enough to generate all known bounds of the forms (2) and (3). Certainly, one can have more complex transformations: for example, the transformation (tv1) may be replaced with

$$f' := \frac{f_1 + f_2 + \cdots + f_c}{c},$$

for $c \in \mathbb{N}$ and $f_i \in B_c$, $i = 1, 2, \ldots, c$. However, this is reflected in the number of bounds generated: the more freedom the transformations have results in the exponentially larger number of bounds.

The complexity of a bound is the number of above transformations applied successively to the starting expression $2x$ in order to get to the final expression (replacements of $x$ with $d_i$ or $m_i$ are not counted in the complexity). We generated 361 bounds of the form (2) with complexity at most 3, and 1138 bounds of the form (3) with complexity at most 2.

### 3.2 Step 2: Testing

In the second step, we refute those of generated conjectured bounds for which we can find a counterexample. For this purpose, we have tested them on the set of all connected graphs with up to 9 vertices, which may be downloaded from Brendan McKay’s web page [27]. (There are more than 273,000 such graphs.
From the same web page one can also download the set of all connected graph on 10 vertices, however—our computational resources did not allow us to test the bounds on this, much larger, set of graphs.

We have also tested the generated bounds for some special graphs which have well suited values of $\mu$, $d_i$ and $m_i$. From the construction, we can easily see that the value of each of the bounds is between $2d_i$ and $2m_i$. If the values of $d_i$ and $m_i$ are close to each other, we cannot have a bound that is much better than a simple and straightforward bound $\mu \leq \max_{v} 2d_i$. Thus, we would like more to test the bounds on graphs which have values of $d_i$ and $m_i$ far apart. Two such graph classes are stars and windmills.

A star $S_n$ is a tree on $n$ vertices having a central vertex of degree $n-1$. For $S_n$ we have $\mu = n$, a central vertex $i$ has $d_i = n-1$ and $m_i = 1$, while the remaining vertices have $d_j = 1$ and $m_j = n-1$, $j \neq i$.

A windmill $W_n$ is a graph on $2n+1$ vertices obtained from $n$ copies of $K_2$ by adding a central vertex adjacent to all other vertices. For $W_n$ we have $\mu = 2n+1$, a central vertex $i$ has $d_i = 2n$ and $m_i = 2$, while the remaining vertices have $d_j = 2$ and $m_j = n+1$, $j \neq i$.

Tests were performed on the total of 273,214 graphs. Among the bounds generated in the first step, 190 of the form (2) and 297 of the form (3) are satisfied for all these graphs. We denote the sets of these bounds by $B_v$ and $B_e$, respectively. These numbers show that the automated way of generating bounds is well chosen, as those that are likely to hold represent a fairly large proportion of all generated bounds. In order to illustrate the wealth of bounds in $B_v$ and $B_e$, we list in Appendix A a sample of them: those in $B_v$ with complexity at most 2 and those in $B_e$ with complexity at most 1.

### 3.3 Step 3: Covering and statistics

In this step we try to answer which bounds among many are worthy of being retained. For each of the sets $B_v$ and $B_e$, we opted to have small subsets $S_v \subseteq B_v$ and $S_e \subseteq B_e$, such that for each test graph $H$ these subsets contain at least one of the bounds which, when evaluated at $H$, gives the smallest value for upper bound on $\mu$.

We use greedy heuristic to find such subsets. We describe it for the set $S_v$, and it is quite analogous for $S_e$.

**Input:** The set of bounds $B_v$ and the set of test graphs $T$.

**Output:** The subset of bounds $S_v$.

1. $S_v := \emptyset$, $B := B_v$, $T := T$
2. while $T \neq \emptyset$
3. for each $f \in B$
4. let $T_f := \{ H \in T : f(H) = \min_{g \in B} g(H) \}$
5. let $t_f := |T_f|$  
6. find $f \in B$ such that $t_f = \max_{g \in B} t_g$
7. $S_v := S_v \cup \{ f \}$, $T := T \setminus T_f$
8. end
Here \( T_f \) represents the number of test graphs \( H \) for which the value of \( f(H) \) is the smallest value for the upper bound on \( \mu \). Thus, in each iteration we put in \( S_v \) the bound which has the smallest value for the largest number of remaining test graphs.

The bounds from \( S_v \) and \( S_e \) are given in Appendix B. There are 17 bounds in \( S_v \) and 31 bounds in \( S_e \). There are plenty of rather complex bounds in this set, as they usually give better values than simple ones.

Note that, in principle, the sets \( S_v \) and \( S_e \) that we have found need not be smallest possible. Namely, each test graph \( H \) defines a set \( S_H \) of bounds achieving the smallest value for an upper bound on \( \mu \), and sets \( S_v \) and \( S_e \) must have nonempty intersection with \( S_H \). This is an example of a covering problem, which is NP-complete. Taking into account that there were more than 273,000 test graphs and either 190 or 297 bounds, we hope it is understandable why we did not try to solve this problem exactly. However, we will shortly see that the sets \( S_v \) and \( S_e \) are indeed the smallest possible.

At last, for each conjectured bound \( f \in B_v \) we determined the following statistics:

- \( sa_f \) is the number of test graphs \( H \) for which
  \[
  f(H) < \min_{g \neq f, g \in B_v} g(H);
  \]

- \( sb_f \) is the number of test graphs \( H \) for which
  \[
  f(H) = \min_{g \in B_v} g(H).
  \]

Thus, in the statistic \( sa_f \) we count test graphs \( H \) for which the value of \( f(H) \) is strictly smaller than the value of \( g(H) \) for any other bound \( g \in B_v \), while in the statistic \( sb_f \) we also admit test graphs \( H \) for which there may be another bound \( g \in B_v \) with \( g(H) = f(H) \).

We determined the same statistics for bounds in \( B_e \). The values of these statistics are given as an ordered pair \((sa_f, sb_f)\) in front of each bound in Appendix B. The bounds are sorted in decreasing order by \( sb_f \). These statistics may serve to illustrate the relative importance of the bounds.

The behaviour of the statistic \( sa_f \) for \( f \in B_v \) is a bit unexpected: it is nonzero for bounds in \( S_v \) and zero elsewhere. Note that a nonzero value of \( sa_f \) means that for each test graph \( H \) for which \( f(H) < \min_{g \in B_v, g \neq f} g(H) \) it holds that \( S_H = \{ f \} \), and thus, the bound \( f \) must belong to \( S_v \). Since the values of bounds in \( S_v \) yield \( \min_{g \in B_v} g(H) \) for all test graphs \( H \), we have proved the following

**Observation 1.** The set \( S_v \) has the smallest cardinality among all subsets of \( B_v \) satisfying that for each test graph \( H \) it holds that

\[
(\exists f \in S_v) \ f(H) = \min_{g \in B_v} g(H). \]
What is unexpected here is that the subset $S_v$, obtained by a greedy heuristic, does not contain bounds from $B_v$ with $sa_f = 0$. The sum of the statistic $sa_f$ for bounds in $S_v$ is equal to 266, 224, which is roughly 97.5% of all test graphs. For the remaining 6990 (or 2.5%) of test graphs, there are always at least two bounds yielding the smallest value for upper bound on $\mu$, one of them always being from $S_v$. For each bound $f \in S_v$ the difference $sb_f - sa_f$ indicates for how many of these 6,990 graphs the bound $f$ is among those yielding the smallest value. Since the sum of the statistic $sb_f$ for bounds in $S_v$ is equal to 306, 513, we can say that, on average, each of these 6,990 graphs has between 5 and 6 bounds yielding the smallest value. Moreover, the difference $sb_f - sa_f$ is largest for bounds No. 2 and 5, as given in Appendix B (6868 and 6521, respectively), meaning that these two bounds give the smallest value for majority of these 6,990 graphs.

The situation with statistics is quite similar for bounds in $B_e$. Once again, the statistic $sa_f$ is nonzero for bounds in $S_e$ and zero elsewhere, implying the following

**Observation 2.** The set $S_e$ has the smallest cardinality among all subsets of $B_e$ satisfying that for each test graph $H$ it holds that

$$\exists f \in S_e \quad f(H) = \min_{g \in B_e} g(H).$$

The sum of the statistic $sa_f$ for bounds in $S_e$ is equal to 267, 555, which is roughly 97.9% of all test graphs. For the remaining 5659 (or 2.1%) of test graphs, there are always at least two bounds yielding the smallest value for upper bound on $\mu$, one of them always being from $S_e$, and on average between 5 and 6 bounds.

### 4 How to prove a few bounds

In this section we present a simple technique, which may be used to prove upper bounds in both forms (2) and (3).

#### 4.1 Bounds of the form (2)

Let $x$ be an eigenvector corresponding to the largest Laplacian eigenvalue $\mu$ of a graph $G$. Let $x_i$ be its component having the largest absolute value. We may suppose that $x_i$ is positive, so that $|x_j| \leq x_i$ for all $j$. A number of bounds have been proven by considering component $x_i$ and the values for the corresponding vertex $v_i$. For example, we have that

$$\mu x = Lx = Dx - Ax,$$

from which it follows that

$$\mu x_i = d_i x_i - \sum_{v_j \sim v_i} x_j \leq d_i x_i + \sum_{v_j \sim v_i} x_i = 2d_i x_i$$
and we may conclude that
\[ \mu \leq \max_{v_i} 2d_i. \]

Similarly,
\[
\mu^2 x = L^2 x = (D - A)^2 x = D^2 x - DAx - ADx + A^2 x
\]
from which it follows that
\[
\mu^2 x_i = d_i^2 x_i - d_i \sum_{v_j \sim v_i} x_j - \sum_{v_j \sim v_i} d_j x_j + \sum_{v_j \sim v_i, v_k \sim v_j} x_k
\]
\[
\leq d_i^2 x_i + d_i \sum_{v_j \sim v_i} x_i + \sum_{v_j \sim v_i} d_j x_j + \sum_{v_j \sim v_i, v_k \sim v_j} x_i
\]
\[
= 2d_i^2 x_i + 2d_i m_i x_i,
\]
and we may conclude that
\[
\mu \leq \max_{v_i} \sqrt{2d_i(d_i + m_i)} \quad \text{(see [25])}.
\]

In general, we may consider a simple quadratic function of \( \mu \):
\[
(\mu^2 + b\mu)x = (D^2 x - DAx - ADx + A^2 x) + b(Dx - Ax)
\]
from which it follows that
\[
(\mu^2 + b\mu)x_i = (d_i^2 x_i - d_i \sum_{v_j \sim v_i} x_j - \sum_{v_j \sim v_i} d_j x_j + \sum_{v_j \sim v_i, v_k \sim v_j} x_k) + b(d_i x_i - \sum_{v_j \sim v_i} x_j)
\]
\[
= (d_i + b)d_i x_i - (d_i + b) \sum_{v_j \sim v_i} x_j - \sum_{v_j \sim v_i} d_j x_j + \sum_{v_j \sim v_i, v_k \sim v_j} x_k
\]
\[
\leq 2(d_i + b)d_i x_i + 2m_i d_i x_i,
\]
provided that \( d_i + b \geq 0 \). We get that
\[
\mu^2 + b\mu - 2d_i(d_i + m_i + b) \leq 0.
\]

From this quadratic inequality it follows that
\[
\mu \leq \frac{-b + \sqrt{b^2 + 8d_i(d_i + m_i + b)}}{2}. \tag{6}
\]
Putting different values for \( b \) we can get various upper bounds. For example,
\[
b = -d_i \quad \Rightarrow \quad \mu \leq \frac{d_i + \sqrt{d_i^2 + 8d_i m_i}}{2} \quad \text{(see [19])}.
\]

We can get similar bounds by considering higher powers of \( L \). However, the bounds so obtained cannot be expressed just in terms of \( d_i \) and \( m_i \), but
they also involve degrees and average degrees of vertices at a specified distance from \( i \). For example, considering \( L^3 \) we get

\[
\mu^3 x_i = \mu^3 x = D^3 x - D^2 A x - D A^2 x + AD^2 x + A D A x + A^2 D x - A^3 x
\]

\[
\mu^3 x_i = d^3_i x_i - d^2_i \sum_{v_j \sim v_i} x_j - d_i \sum_{v_j \sim v_i} d_j x_j + d_i \sum_{v_j \sim v_i} \sum_{v_k \sim v_j} x_k - \sum_{v_j \sim v_i} d^2_j x_j
\]

\[
+ \sum_{v_j \sim v_i} d_j \sum_{v_k \sim v_j} x_k + \sum_{v_j \sim v_i} \sum_{v_k \sim v_j} d_k x_k - \sum_{v_j \sim v_i} \sum_{v_k \sim v_j} \sum_{v_l \sim v_k} x_l
\]

\[
\leq 2(d^3_i + d^2_i m_i + \sum_{v_j \sim v_i} d^2_j + \sum_{v_j \sim v_i} d_j m_j) x_i,
\]

from which it follows that

\[
\mu \leq \max_{v_i} \sqrt{2d^2_i (d_i + m_i) + 2 \sum_{v_j \sim v_i} d_j (d_j + m_j)}.
\]

Starting with these bounds that hold for \( v_i \), we can prove a number of similar bounds using various means. Namely, if \( f_j(x, y), j = 1, 2, \ldots, k \), are functions such that

\[
\mu \leq f_j(d_i, m_i), \quad j = 1, 2, \ldots, k,
\]

then a mean of these functions satisfies the same inequality, i.e., for \( c_j \geq 0 \), \( j = 1, 2, \ldots, k \), such that \( \sum_{j=1}^k c_j = 1 \), we have that:

(a) (Arithmetic mean)

\[
\mu \leq \sum_{j=1}^k c_j f_j(d_i, m_i);
\]

(b) (Geometric mean)

\[
\mu \leq \prod_{j=1}^k f_j(d_i, m_i)^{c_j};
\]

(c) (Square mean)

\[
\mu \leq \sqrt[k]{\sum_{j=1}^k c_j f_j(d_i, m_i)^2};
\]

(d) (Harmonic mean)

\[
\mu \leq \frac{1}{\sum_{j=1}^k c_j \left( \frac{c_j}{f_j(d_i, m_i)} \right)}.
\]

For example, from \( \mu \leq 2d_i \) and \( \mu \leq \sqrt{2d_i(d_i + m_i)} \) we get, using geometric mean with \( c_1 = \frac{1}{3} \) and \( c_2 = \frac{2}{3} \), that

\[
\mu \leq \sqrt[3]{4d^2_i(d_i + m_i)}.
\]
It should be noted here that all these average bounds are dominated by a set of bounds \( \mu \leq \max_{v_i} f_j(d_i, m_i), \quad j = 1, 2, \ldots, k \). Further, each of these bounds is weaker than the bound

\[
\mu \leq \min_{j=1,2,\ldots,k} f_j(d_i, m_i),
\]

but, unfortunately, in most cases this bound does not have an explicit form.

### 4.2 Bounds of the form (3)

Similar results can be obtained for bounds of this type. Let \( G^* \) be the line graph of \( G \) having an adjacency matrix \( A^* \) and let \( \lambda^* \) be the largest eigenvalue of \( A^* \). We will denote ends of an edge \( e \) of \( G \) by \( e_1 \) and \( e_2 \). For example, the degree of a vertex \( e \) in \( G^* \) is equal to \( d_{e_1} + d_{e_2} - 2 \). It was recently shown in [33, Lemma 2] that for any connected graph \( G \) the relation \( \mu \leq \lambda^* + 2 \) holds, with equality if and only if \( G \) is bipartite.

Let \( x \) be an eigenvector corresponding to the largest eigenvalue \( \lambda^* \) of \( A^* \). Let \( x_e \) be its component having the largest absolute value. We may suppose that \( x_e \) is positive, so that \( |x_f| \leq x_e \) for all \( f \). We can prove a few bounds by considering component \( x_e \) and the values for the corresponding edge \( e \).

First, we have that

\[
\mu x_e \leq (\lambda^* + 2)x_e = ((A^* + 2I)x)_e = \sum_{f \sim e} x_f + 2x_e \leq \sum_{f \sim e} x_f + 2x_e = (d_{e_1} + d_{e_2})x_e,
\]

from which it follows that

\[
\mu \leq d_{e_1} + d_{e_2} \leq \max_{\{v_i, v_j\} \in E} d_i + d_j \quad \text{ (see [1]).}
\]

On the other hand, we have that

\[
\mu^2 x_e \leq (\lambda^* + 2)^2 x_e = ((A^* + 2I)^2 x)_e = ((A^*)^2 + 4A^* + 4I)x_e
\]

\[
= \sum_{f \sim e} \sum_{g \sim f} x_g + 4 \sum_{f \sim e} x_f + 4x_e
\]

\[
\leq \sum_{f \sim e} \sum_{g \sim f} x_e + 4 \sum_{f \sim e} x_e + 4x_e
\]

\[
= \sum_{f \sim e} (d_{f_1} + d_{f_2} - 2)x_e + 4(d_{e_1} + d_{e_2} - 2)x_e + 4x_e
\]

\[
= \sum_{f_2 \sim e_1, f_2 \neq e_2} (d_{e_1} + d_{f_2} - 2)x_e + \sum_{f_2 \sim e_2, f_2 \neq e_1} (d_{e_2} + d_{f_2} - 2)x_e
\]

\[
+ 4(d_{e_1} + d_{e_2} - 1)x_e
\]

\[
= (d_{e_1} - 1)(d_{e_1} - 2)x_e + (d_{e_1} m_{e_1} - d_{e_1})x_e
\]

\[
+ (d_{e_2} - 1)(d_{e_2} - 2)x_e + (d_{e_2} m_{e_2} - d_{e_2})x_e
\]

\[
+ 4(d_{e_1} + d_{e_2} - 1)x_e
\]

\[
= (d_{e_1}^2 + d_{e_1} m_{e_1} + d_{e_2}^2 + d_{e_2} m_{e_2})x_e.
\]
from which it follows that
\[ \mu \leq \max_{(v_i,v_j) \in E} \sqrt{d_i^2 + d_i m_i + d_j^2 + d_j m_j} \quad \text{(see [35]).} \]

As in the previous subsection, we can consider a quadratic function of \( \mu \) in order to get more general bounds:
\[
(\mu^2 + b \mu) x_e = \sum_{f \sim e} \sum_{g \sim f} x_g + 4 \sum_{f \sim e} x_f + 4 x_e + b( \sum_{f \sim e} x_f + 2 x_e )
\]
\[
= \sum_{f \sim e} \sum_{g \sim f} x_g + (b + 4) \sum_{f \sim e} x_f + (2b + 4) x_e
\]
\[
\leq \sum_{f \sim e} \sum_{g \sim f} x_e + (b + 4) \sum_{f \sim e} x_e + (2b + 4) x_e
\]
\[
= (d_{e_1}^2 + d_{e_1} m_{e_1} + d_{e_2}^2 + d_{e_2} m_{e_2}) x_e + b(d_{e_1} + d_{e_2}) x_e,
\]
provided that \( b + 4 \geq 0 \). We have
\[
\mu^2 + b \mu - (d_{e_1}^2 + d_{e_1} m_{e_1} + d_{e_2}^2 + d_{e_2} m_{e_2} + b(d_{e_1} + d_{e_2})) \leq 0,
\]
therefore
\[
\mu \leq \frac{-b + \sqrt{b^2 + 4(b(d_{e_1} + d_{e_2}) + 4(d_{e_1}^2 + d_{e_1} m_{e_1} + d_{e_2}^2 + d_{e_2} m_{e_2}))}}{2}
\]
\[
= \frac{-b + \sqrt{(b + 2d_{e_1} + 2d_{e_2})^2 - 8d_{e_1} d_{e_2} + 4d_{e_1} m_{e_1} + 4d_{e_2} m_{e_2}}}{2}.
\]
Substituting various values of \( b \), we can get a number of bounds of form (3). For example,
\[
b = -4 \quad \Rightarrow \quad \mu \leq 2 + \sqrt{d_{e_1}(d_{e_1} + m_{e_1} - 4) + d_{e_2}(d_{e_2} + m_{e_2} - 4)} + 4 \quad \text{(see [35]).}
\]
Similarly, we can get further bounds by considering higher powers of \( A^* \) or by using means of the existing bounds.

5 Conclusions

We have explored automated ways to generate two large sets of conjectured upper bounds on the largest Laplacian eigenvalue of graphs. These conjectured bounds hold for all connected graphs with up to 9 vertices, and for that class of graphs, the conjectured bounds are tight, with none being dominated by another.

While the exemplary bounds, mentioned in the introductory section, could be proved, the remaining bounds given in the appendix are open problems. However, instead of proving just one or two of them by hand, it would be much more beneficial to find an approach that would enable proving a substantial number of these bounds.
An important consequence of our study is that, at least empirically shown, there is a strong relation between the largest Laplacian eigenvalue and the degrees in a graph. We believe that similar relations exist between the degrees and other extremal nontrivial eigenvalues of a graph, i.e., the smallest positive Laplacian eigenvalue and the largest and the smallest adjacency matrix eigenvalues. The approach of this paper could most probably be extended to apply to different forms of bounds and different invariants. This would be the object of future work.

Acknowledgement Authors are grateful to Mustapha Aouchiche, who tested correctness of some of the conjectures using AutoGraphiX. We are grateful to the anonymous referee for helpful remarks which led to better presentation and introduction of bound statistics.

For calculation of eigenvalues we have used Colt library [6]. For storing test graphs, their eigenvalues and generated bounds in a database we have used Microsoft SQL Server 2000. On request, all generated data can be obtained from the first author.

References


Appendix A: Bounds of small complexity

Bounds of the form (2) with complexity at most 2, satisfied by all connected graphs on up to 9 vertices and a few stars and windmills:
1. $\max_{v \in V} 2d_v$
2. $\max_{v \in V} m_v + d_v$
3. $\max_{v \in V} \frac{2m_v^2}{d_v}$
4. $\max_{v \in V} \frac{2d_v^2}{m_v}$
5. $\max_{v \in V} \sqrt{\frac{m_v^2 + 3d_v^2}{m_v}}$
6. $\max_{v \in V} \sqrt{\frac{m_v^2}{2m_v} + 3d_v}$
7. $\max_{v \in V} \sqrt{\frac{m_v^2 + 3d_v}{2m_v}}$
8. $\max_{v \in V} \sqrt{\frac{m_v^2 + 3d_v}{m_v}}$
9. $\max_{v \in V} \sqrt{\frac{m_v^2 + 3d_v}{m_v}}$
10. $\max_{v \in V} \sqrt{\frac{4d_v^2}{m_v}}$
11. $\max_{v \in V} \sqrt{\frac{4d_v^2}{m_v}}$
12. $\max_{v \in V} \sqrt{\frac{d_v^2}{m_v} + m_v}$
13. $\max_{v \in V} \frac{m_v^2}{d_v} + m_v$
14. $\max_{v \in V} \frac{d_v^2}{m_v} + m_v$
15. $\max_{v \in V} \frac{d_v^2}{m_v} + d_v$
16. $\max_{v \in V} \frac{m_v^2}{d_v} + 3d_v$
17. $\max_{v \in V} \frac{m_v^2}{d_v} + 3d_v$
18. $\max_{v \in V} \frac{m_v^2}{d_v} + 3d_v$
19. $\max_{v \in V} \frac{2m_v^2}{d_v}$
20. $\max_{v \in V} \frac{2d_v^2}{m_v}$

Bounds of the form (3) with complexity at most 1, satisfied by all connected graphs on up to 9 vertices and a few stars and windmills:

1. $\max_{i, j \sim v} d_i + d_j$
2. $\max_{i, j \sim v} 2(d_i + d_j) - (m_i + m_j)$
3. $\max_{i, j \sim v} \frac{2d_i^2 + d_j^2}{d_i + d_j}$
4. $\max_{i, j \sim v} \frac{2d_i^2 + d_j^2}{m_i + m_j}$
5. $\max_{i, j \sim v} \frac{2(m_i^2 + m_j^2)}{d_i + d_j}$
6. $\max_{i, j \sim v} \sqrt{2(d_i^2 + d_j^2)}$
7. $\max_{i, j \sim v} 2 + \sqrt{2(d_i^2 + d_j^2) - 4(d_i + d_j)} + 4$
8. $\max_{i, j \sim v} 2 + \sqrt{2(d_i^2 + d_j^2) - 4(m_i + m_j)} + 4$

Appendix B: Bounds in $S_v$ and $S_e$

Bounds in $S_v$:

1. (102710, 105371) $\max_{v \in V} \sqrt{5d_v^2 + 11m_v^2}$
2. (56389, 63257) $\max_{v \in V} m_v + d_v$
3. (41770, 43132) $\max_{v \in V} \sqrt{\frac{2m_v^2}{d_v} + 2d_v^2}$
4. (33011, 36696) $\max_{v \in V} \sqrt{\frac{4d_v^2}{m_v} + 12d_v + m_v}$
5. (17832, 24353) $\max_{v \in V} \sqrt{\frac{3d_v^2 + 3m_v^2}{d_v}}$
6. (12366, 14825) $\max_{v \in V} \sqrt{\frac{3d_v^2}{m_v} + 3m_v^2}$
7. (1056, 4198) $\max_{v \in V} \sqrt{2d_v^2 + 14d_v + m_v}$
8. (1056, 4198) $\max_{v \in V} \sqrt{2d_v^2 + 14d_v + m_v}$
Bounds in $S_v$:

1. $(114958, 118179)$ \[ \max_{v_i \sim v_j} \sqrt{d_i^2 + 3d_v m_v} \]
2. $(71269, 74872)$ \[ \max_{v_i \sim v_j} \sqrt{2((m_i - 1)^2 + (m_j - 1)^2) + (d_i^2 + d_j^2) - (d_i m_i + d_j m_j)} \]
3. $(68171, 71725)$ \[ \max_{v_i \sim v_j} 2 + (m_i + m_j - (d_i + d_j) + \sqrt{2(d_i^2 + d_j^2) - 4(m_i + m_j) + 4} \]
4. $(6541, 8260)$ \[ \max_{v_i \sim v_j} \sqrt{d_i^2 + d_j^2 + 2m_i m_j} \]
5. $(3086, 4306)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{3(m_i^2 + m_j^2) - 2m_i m_j - 4(d_i + d_j) + 4} \]
6. $(1404, 3019)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{2((d_i - 1)^2 + (d_j - 1)^2 + m_i m_j - d_i d_j) \]
7. $(268, 1700)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{(d_i - d_j)^2 + 2(d_i m_i + d_j m_j) - 4(m_i + m_j) + 4} \]
8. $(88, 1468)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{d_i^2 + d_j^2 + d_i m_i + d_j m_j - 4(d_i + d_j) + 4} \]
9. $(58, 1324)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{2(d_i^2 + d_j^2) - 16\frac{d_i d_j}{m_i + m_j} + 4} \]
10. $(2, 1275)$ \[ \max_{v_i \sim v_j} \sqrt{d_i^2 + d_j^2 - (m_i - m_j)^2} \]
11. $(4, 1195)$ \[ \max_{v_i \sim v_j} \sqrt{2(d_i^2 + d_j^2)} \]
12. $(520, 1117)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{2(m_i^2 + m_j^2) + (d_i - d_j)^2 - 4(d_i + d_j) + 4} \]
13. $(335, 1025)$ \[ \max_{v_i \sim v_j} \sqrt{d_i^2 + d_j^2 + m_i m_j - d_i d_j} \]
14. $(6, 981)$ \[ \max_{v_i \sim v_j} 2(m_i + m_j) - 4\frac{m_i m_j}{m_i + m_j} \]
15. $(23, 919)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{8(m_i^2 + m_j^2) - 8(d_i^2 + d_j^2) + 4 - 4(d_i + d_j) + 6} \]
16. $(2, 788)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{8(m_i^2 + m_j^2) - 8(d_i m_i + d_j m_j) + 4 - 4(d_i + d_j) + 6} \]
17. $(287, 776)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{2(m_i^2 + m_j^2) + (d_i m_i + d_j m_j) - (d_i^2 + d_j^2) - 4(d_i + d_j) + 4} \]
18. $(92, 570)$ \[ \max_{v_i \sim v_j} 2 + \sqrt{3(m_i^2 + m_j^2) - (d_i^2 + d_j^2) - 4(m_i + m_j) + 4} \]
19. $(288, 526)$ \[ \max_{v_i \sim v_j} \frac{(d_i^2 + d_j^2)(m_i + m_j)}{2d_i d_j} \]
20. $\max_{v_i \sim v_j} 2 + \sqrt{2(m_i^2 + m_j^2) - 8 \frac{d_i^2 + d_j^2}{m_i + m_j} + 4}$

21. $\max_{v_i \sim v_j} 2 + \sqrt{2(m_i^2 + m_i m_j + m_j^2) - (d_i m_i + d_j m_j) - 4(d_i + d_j) + 4}$

22. $\max_{v_i \sim v_j} \frac{2(m_i^2 + m_i m_j + m_j^2) - (d_i^2 + d_j^2)}{m_i + m_j}$

23. $\max_{v_i \sim v_j} 2 + \sqrt{2(m_i^2 + m_i m_j + m_j^2) - (d_i^2 + d_j^2) - 4(d_i + d_j) + 4}$

24. $\max_{v_i \sim v_j} \frac{2(m_i^2 + m_j^2)}{2 + \sqrt{2(d_i - 1)^2 + (d_j - 1)^2}}$

25. $\max_{v_i \sim v_j} 2 + \sqrt{m_i^2 + 4m_i m_j + m_j^2 - 2d_i d_j - 4(d_i + d_j) + 4}$

26. $\max_{v_i \sim v_j} \frac{d_i + d_j + m_i + m_j - 4 \frac{d_i d_j}{m_i + m_j}}{d_i d_j}$

27. $\max_{v_i \sim v_j} \frac{m_i m_j (d_i + d_j)}{d_i d_j}$

28. $\max_{v_i \sim v_j} \frac{(m_i + m_j)(d_i m_i + d_j m_j)}{2m_i m_j}$

29. $\max_{v_i \sim v_j} \frac{m_i^2 + 4m_i m_j + m_j^2 - (d_i m_i + d_j m_j)}{d_i d_j}$

30. $\max_{v_i \sim v_j} \frac{(m_i + m_j)(d_i m_i + d_j m_j)}{2d_i d_j}$

31. $\max_{v_i \sim v_j} 2 + \sqrt{(m_i - m_j)^2 + 4d_i d_j - 4(m_i + m_j) + 4}$