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A survey of automated conjectures in spectral graph theory

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ABSTRACT

During the last three decades, the computer has been widely used in spectral graph theory. Many results about graph eigenvalues were first conjectured, and in some cases proved, using computer programs, such as GRAPH, Graffiti, Ingrid, newGRAPH and AutoGraphiX. This paper presents a survey and a discussion of such results.

1. Introduction

Computers have long been used in evaluating eigenvalues and eigenvectors of matrices in general and graph related matrices, thus in spectral graph theory, in particular. But the role of computers in spectral graph theory, and graph theory in general [69], is not limited to evaluations. Indeed, computers can also be used to advance the theory *per se*, *i.e.,* to provide conjectures, refutations and proofs (or ideas of proofs).

While only a few attempts have been made at full automation of proofs in spectral graph theory [33, 35], partial automation of complex proofs has been fruitful. Much work has been devoted to assisted, or in some cases, automated discovery of conjectures in spectral graph theory. This was first done in an interactive way by Cvetković and his collaborators [33,35] with the system GRAPH. Later, in a more automated way many conjectures were obtained by Fajtlowicz [42,49,50] with the system Graffiti and by Aouchiche et al. [2,4–6,18,20,21] with the system AutoGraphiX (AGX for short). A few relations

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were obtained by Brigham et al. [13,14,15] with the system Ingrid and in a similar vein by Gernert [59]. Further results were recently obtained by Colton [26] with the system HR and by Stevanović with the system newGRAPH (available at "www.mi.sanu.ac.yu/newgraph/") as well as with an unnamed specialized system [12]. Other systems which appear to have the potential to find relations in spectral graph theory are Graffiti.pc, due to Delavina [41], GraPHedron, due to Mélot [24,84], and GrInvIn, due to Peeters et al. [101].

The system GRAPH, an interactive programming package and an expert system for graph theory, was developed at University of Belgrade, Faculty of Electrical Engineering, during the period 1980–1984 by Dragoš Cvetković and his collaborators. Basic references about the system are [28,33,35,37]. It was extensively used to find conjectures and prove theorems in graph theory (usually the latter only being published), with an emphasis on spectral graph theory. GRAPH comprises three components.

- A bibliographic component, BIBLI, devoted to bibliographic data processing: it allows storage and retrieval of information on papers, books, proceedings, reports, abstracts, manuscripts and documents.
- An algorithmic component, ALGOR, directly connected to the conjecture-making task [32, p. 20]:

  "The part of the system "GRAPH" described is primarily meant as a means for quick[ly] checking, disproving or making conjectures in graph theory. Facilities provided by the system enable to get the answer on a great number of questions on graphs of a reasonable size in a few seconds (of course, what does a reasonable size mean depends on the problem considered)."

  Results of GRAPH consist of computer-assisted conjectures, refutations and proofs. Most of the published results are theorems, and while mention of system GRAPH is made, details on how it led interactively to conjectures, refutations or proofs are unfortunately not given except in [32] (automated theorem-proving is discussed in more detail [27,33]).
- An automated theorem proving one, THEOR, designed for computer-assisted or automated theorem-proving in (spectral) graph theory, and is described in Cvetković and Pevac [33]. It contains point variables, line variables, integer variables, graph names, constraints, function names, operations over graphs and predicates. The effectiveness of the prover depends largely on a set of lemmas which represent beginner's knowledge of graph theory. The user may select more advanced lemmas.

Graffiti generates many conjectures of a simple form (e.g. inequalities between two invariants or between an invariant and the sum of two others) then tests them on a database of graphs and discards those which are falsified. Should this test be passed, it is checked if the formulas are implied by known ones (in which case they are also discarded) and that they provide new information for at least one graph in the database, *i.e.*, that they are stronger than the conjunction of all other formulas for that graph. If not, they are temporarily set aside. If yes, they are proposed to all graph theorists, in the electronic file "Written on the Wall" [50], which reports on the status of almost 1000 conjectures. Many well-known graph theorists worked on these conjectures and this led to several dozen papers. Some of Graffiti's conjectures are about various topics in spectral graph theory, namely, the eigenvalues, as well as their multiplicity, of the adjacency, Laplacian and distance matrices of graphs.

The Ingrid system of Brigham and Dutton [13–15], manipulates formulas on graph invariants from a database to compute bounds on some invariants when others are limited to some range. At the beginning, the system used a database of 36 graph invariants described by about 350 theorems. It is based on about 1200 chaining rules to detect, by transitivity, possible relations between the 36 invariants. Among the objectives, starting from bounds stated in known results, Ingrid determines better upper and lower bounds on some invariants as functions of other invariants. Ingrid can be used to

- help solve practical problems,
- derive new theorems (by selecting relations leading to them),

- test the effectiveness of new theorems (by showing they are or not consequences of one or several previously known ones),
- test conjectures (viewed as "temporary theorem" to see if this implies some contradiction),
- resolve open problems (by showing they imply some contradiction), and
- help to study graph theory.

The system newGRAPH (available at http://www.mi.sanu.ac.yu/newGRAPH/) retains the spirit of GRAPH, but uses more sophisticated tools in order to provide a more "user-friendly" work environment. Above all, newGRAPH is modular and adaptive to the needs of a specific researcher. Using the concept of plug-ins and an extensive library, the user is able to write his/her own graph invariants, graph generators and graph actions or import existing ones. A spectral graph theorist often encounters the need for the simultaneous editing of two or more interdependent graphs (e.g. a graph and its line graph), together with multiple labellings of their vertices and edges. Occasionally, labellings are of such kind that it could be beneficial to permit the user to modify the labeling and test whether it still satisfies a given property. Such tasks are implemented in the system newGRAPH.

The AutoGraphiX (AGX) system was developed at GERAD, Montreal since 1997. It addresses the following problems:

- Find a graph G satisfying given constraints;
- Find a graph G maximizing or minimizing a given invariant, possibly subject to constraints;
- Find a conjecture, which may be algebraic, *i.e.,* a relation between graph invariants, or structural, *i.e.,* a characterization of extremal graphs for some invariant;
- Corroborate, refute and/or strengthen or repair a conjecture;
- Suggest ideas of proof.

The AGX system was described in [4,20]; three ways it uses to fully automate conjecture making are presented in [21]. Applications to spectral graph theory are given in [2,3,10,19,38,70,72,114,115]. The main ideas behind AGX are that

- all problems listed above can be expressed as parametric constrained optimization ones on an infinite family of graphs, and
- a *generic* heuristic can be used for solving all of them.

More precisely, letting $i(G)$ denote an invariant of G, or a formula involving several invariants which is itself an invariant, $\mathcal{G}_n$ the set of all graphs with n vertices, $\mathcal{G}_{n,m}$ the set of all graphs with n vertices and m edges (we may also consider any graph invariant as a parameter), one solves heuristically the problem

$$Min/Max \quad \{i(G), G \in \mathcal{G}_n\} \quad \text{or} \quad Min/Max \quad \{i(G), G \in \mathcal{G}_{n,m}\}.$$

In practice only moderate values of n and m will be considered.

The principle of AGX is to use heuristic optimization to find a family of extremal or near-extremal graphs for some objective, subject to constraints, then to exploit the corresponding information.

Heuristic optimization in AGX follows the Variable Neighborhood Search (VNS) metaheuristic [71, 91], or framework for building heuristics. VNS exploits the idea of systematic change of neighborhood within the search. This is done in two ways: first in a descent routine, called Variable Neighborhood Descent (VND), which leads to a local optimum, and, second, in a systematic effort to get away from this local optimum by applying increasingly strong perturbations and descents.

2. Adjacency matrix

Let $G = (V, E)$ a simple graph on n vertices. The adjacency matrix A of G is defined by its entries $a_{ij} = 1$ if $ij \in E$ and 0 otherwise. The spectrum of the adjacency matrix of G is also called the spectrum

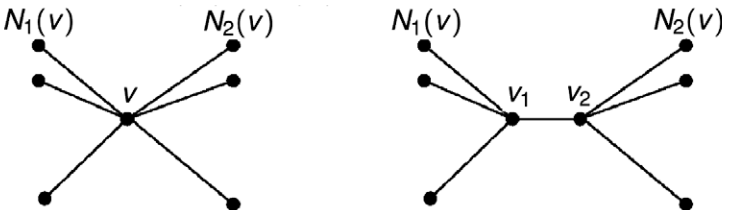

Fig. 1. Splitting v to v_1 and v_2 with respect to $N_1(v)$ and $N_2(v)$.

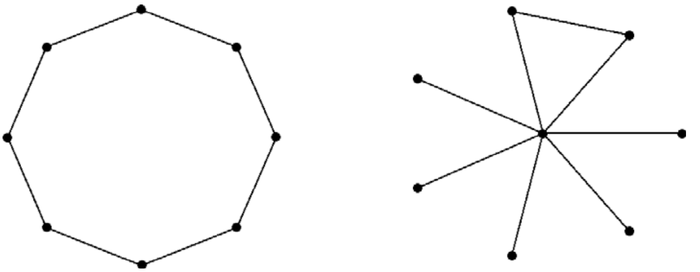

Fig. 2. The unicyclic graphs C_8 and S_8^+.

of G and denoted $(\lambda_1, \lambda_2, \ldots, \lambda_n)$. The eigenvalues of G are labelled such that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. The largest eigenvalue λ_1 is called the spectral radius or the index of G.

In this section, we survey some results related to the spectrum of a graph first obtained by the use of a computer program (among those presented in Section 1 above). A subsection is devoted to each of the largest (index), second largest and smallest eigenvalues, respectively. A few results related to the positive and negative eigenvalues are given in the fourth subsection. Therefore results involving the energy of graph (defined below) are recalled. To end the section, we summarize the results about integral graphs obtained using the computer program newGRAPH.

2.1. The index

We list a couple of results obtained with GRAPH, see [35] for a more comprehensive set. Let G be a graph, v a distinguished vertex, and $N_1(v)$, $N_2(v)$ a partition of the neighbors of v. If G' is obtained from $G - v$ by adding vertices v_1, v_2 and edges $\{v_1, w\}$ with $w \in N_1(v)$ and $\{v_1, w\}$ with $w \in N_2(v)$, G' is obtained by *splitting* vertex v (see Fig. 1). The following result was conjectured with the system GRAPH and proved in [110]:

Theorem 1. *If G is a connected graph and G' is obtained from G by splitting a vertex, then $\lambda_1(G') < \lambda_1(G)$, where $\lambda_1(G)$ is the index of G or the largest eigenvalue of its adjacency matrix.*

A connected graph is said to be *unicyclic* if it contains exactly one cycle. Let C_n denote the cycle on n vertices and S_n^+ the graph obtained from the star S_n on n vertices by adding an edge (see Fig. 2 for C_8 and S_8^+). Obviously, both C_n and S_n^+ are unicyclic graphs. The following theorem is obtained by GRAPH.

Theorem 2. *Let G be a unicyclic graph on n vertices with index λ_1. Then*

$$\lambda_1(C_n) \leqslant \lambda_1 \leqslant \lambda_1(S_n^+)$$

with equality if and only if G is C_n for the lower bound and if and only if G is S_n^+ for the upper bound.

Denote by $\rho(k)$ the largest eigenvalue of the graph obtained from the cycle C_n with $n \geqslant 6$ by adding an edge between two vertices at distance $k = 2, 3, \ldots, \lfloor n/2 \rfloor$. On the basis of experiments conducted with GRAPH it was conjectured that $\rho(k)$ is monotonous and decreases. This was proved in [106,111].

The chromatic number $\chi = \chi(G)$ of a graph G is the minimum number of colors needed to color the vertices of a graph such that no two adjacent vertices have the same color. A clique in a graph G is a set of mutually adjacent vertices. The number of vertices in a largest clique in G is called the clique number of G and denoted by $\omega = \omega(G)$.

Among the invariants available in Ingrid, there is the index or the spectral radius λ_1 of a graph (it is, in fact the only spectral graph invariant in Ingrid). The system reproduced [13] the following inequality, first proved in [29],

$$\chi \geqslant \frac{n}{n - \lambda_1},$$

where n and χ denote respectively the order and the chromatic number of a graph. Two other reproduced inequalities, first proved in [48], are the following

$$\omega \geqslant \frac{n}{n - \lambda_1} - \frac{1}{3} \quad \text{and} \quad \chi \geqslant \frac{2m}{2m - \lambda_1^2},$$

where m and ω are respectively the size (number of edges) and the maximum clique number of the graph.

As said above, Ingrid can be used to test the effectiveness of a theorem. For instance, the bound $\lambda_1 \leqslant \left(-1 + \sqrt{1 + 8m}\right) \big/ 2$, due to Stanley [113], is found to be a consequence of the following two inequalities $\lambda_1 \leqslant \sqrt{2m(\chi - 1)/\chi}$ and $\chi \leqslant \left\lfloor 1 + \sqrt{1 + 2m} \right\rfloor$, both available in the system database.

A subset S of vertices of G is a dominating set if each vertex of G is in S or adjacent to at least a vertex from S. The minimum size of a dominating set in G is called the domination number of G and denoted by $\beta = \beta(G)$.

Another type of problem related to the index $\lambda_1(G)$ of a graph G is to find its extremal values when a given graph invariant is fixed. This kind of problem is mainly studied using the AGX system. To illustrate, consider the problem of finding the maximum value of the index of graphs on n vertices with given domination number β, *i.e.*,

$$Max \quad \{\lambda_1(G), G \in \mathcal{G}_{n,\beta}\},$$

where $\mathcal{G}_{n,\beta}$ is the set of all connected graphs on n vertices with domination number β (n and β are, then, parameters). This problem was studied using AGX and conjectures obtained were proved in [114]. Before the statement of the theorem, let us recall some definitions. For two graphs G and H, the union graph $G \cup H$ is the graph defined on the vertex set $V = V_G \cup V_H$ and the edge set $E = E_G \cup E_H$, while kG denotes the union of k copies of G. The *surjective split graph* $SSG(n, k; a_1, \ldots, a_k)$, defined for positive integers $n, k, a_1, \ldots, a_k$, with $n \geqslant k \geqslant 3$, satisfying $a_1 + \cdots + a_k = n - k$, $a_1 \geqslant a_2 \geqslant \cdots \geqslant a_k$, is a split graph on n vertices formed from a clique K with $n - k$ vertices and an independent set I with k vertices, in such a way that the ith vertex of I is adjacent to a_i vertices of K, and that no two vertices of I have a common neighbor in K. See Fig. 3 for examples of surjective split graphs. Note that $\beta(SSG(n, k; a_1, \ldots, a_k)) = k$.

Theorem 3. *If G is a connected graph on n vertices with domination number β, then*

(1) *if $\beta = 1$, then $\lambda_1(G) \leqslant \lambda_1(K_n) = n - 1$, with equality if and only if $G \cong K_n$;*
(2) *if $\beta = 2$ and n is even, then $\lambda_1(G) \leqslant \lambda_1\left(\overline{\frac{n}{2}K_2}\right)$, with equality if and only if $G \cong \overline{\frac{n}{2}K_2}$;*
(3) *if $\beta = 2$ and n is odd, then $\lambda_1(G) \leqslant \lambda_1\left(\overline{\left(\frac{n-1}{2} - 1\right) K_2 \cup P_3}\right)$, with equality if and only if $G \cong \overline{\left(\frac{n-1}{2} - 1\right) K_2 \cup P_3}$;*
(4) *if $3 \leqslant \beta \leqslant \frac{n}{2}$, then $\lambda_1(G) \leqslant \lambda_1(SSG(n, \beta; n - 2\beta + 1, 1, 1, \ldots, 1))$, with equality if and only if $G \cong SSG(n, \beta; n - 2\beta + 1, 1, 1, \ldots, 1)$.*

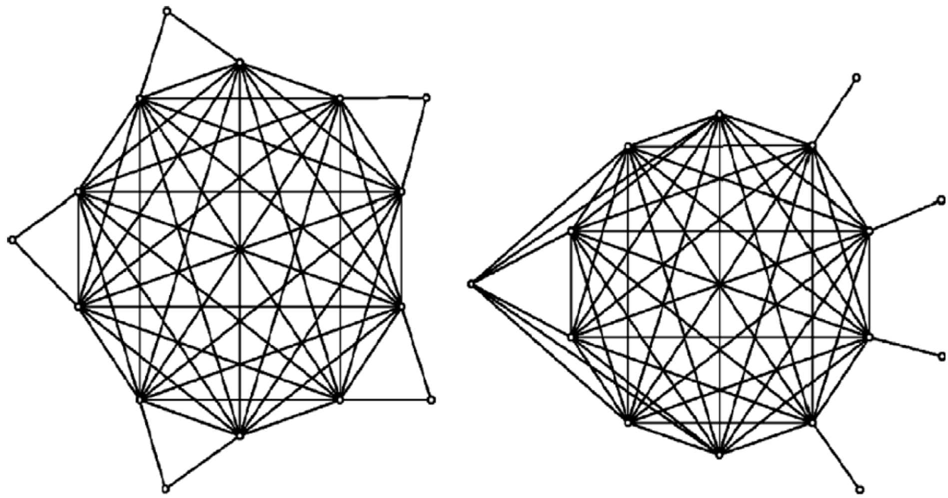

Fig. 3. Examples of surjective split graphs.

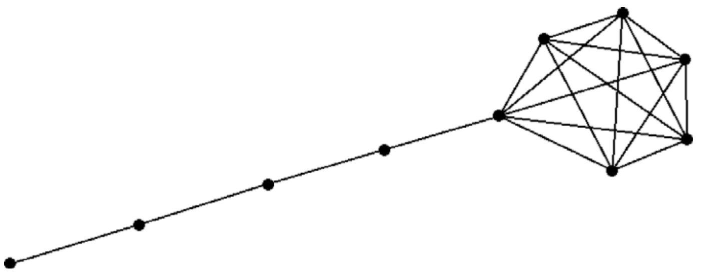

Fig. 4. The kite $Ki_{10,6}$.

Similarly, the problem of finding the extremal graphs for λ_1 when the clique number is fixed was studied using again the AGX system. The results are gathered in [116], where the main theorem is the following. First, recall that a kite $Ki_{n,\omega}$ is the graph obtained from a clique K_ω and a path $P_{n-\omega}$ by adding an edge between a vertex from the clique and an endpoint from the path (see Fig. 4 for $Ki_{10,6}$).

Theorem 4. *Let G be a connected graph on n vertices with clique number ω. Then*

$$\lambda_1(G) \geqslant \lambda_1(Ki_{n,\omega})$$

with equality if and only if G is isomorphic to the kite $Ki_{n,\omega}$.

An automated comparison of 20 graph invariants [2,5] was done using the system AGX. The results and/or conjectures were of the following form (called *AGX Form* 1). For all connected graphs $G = (V, E)$ with $n = |V|$, find conjectures of the form

$$l_n \leqslant i_1(G) \oplus i_2(G) \leqslant u_n, \tag{1}$$

where $i_1(G)$ and $i_2(G)$ are invariants; $\oplus$ is one of the four operations $+, -, \times, /$; l_n and u_n are lower and upper bounding functions of the order n of G which are *best possible, i.e.*, such that for each value of n (except possibly very small ones where border effects appear) there is a graph G for which the bound is tight.

Table 1
Statistics for AGX Form 1 conjectures about λ_1.

Results type	Number of results	%
Known results	7	4.61
Automated proof	68	44.74
Proved by hand	23	15.13
Open (complete) conjectures	23	15.13
Structural open conjectures	16	10.52
Refuted conjectures	5	3.29
No result	10	6.58

Note that this form extends that of the well-known Nordhaus–Gaddum [99] relations in that

- $i_1(G)$ and $i_2(G)$ are two different invariants instead of $i_2(G)$ being equal to $i_1(\overline{G})$, where $\overline{G}$ is the complementary graph of G (in which an edge joins vertices u and v if and only if no edge does so in G);
- operations $-$ and/are considered in addition to $+$ and $\times$.

In 148 cases (296 bounds) over the 760 possible results of the AGX Form 1, a spectral graph theory invariant is involved. Indeed, the index λ_1 of a graph was compared with 19 invariants and the algebraic connectivity was compared with 18 invariants (19, including λ_1). Among these 296 bounds, several known results were reproduced, such as $\lambda_1 \geqslant \delta$, $\lambda_1 \geqslant \overline{d}$, $\lambda_1 \leqslant \Delta$ and $\lambda_1 \geqslant \chi - 1$, where δ, $\overline{d}$, Δ and χ denote the minimum, average, and maximum degree, and the chromatic number respectively. The following (new) results are among the outcome of the automated comparison.

Proposition 5 [2]. *For any connected graph G on $n \geqslant 2$ vertices with index λ_1 and chromatic number χ,*

$$\frac{\lambda_1}{\chi} \leqslant \frac{1}{2}\sqrt{\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil},$$

with equality if and only if G is the balanced complete bipartite graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

The distance $d(u, v) = d_G(u, v)$ between two vertices u and v in a connected graph G is the length of a shortest path between u and v. The average distance in G is denoted by $\overline{l} = \overline{l}(G)$. The maximum distance between two vertices is the diameter $D = D(G)$. The eccentricity $ecc(v) = ecc_G(v)$ of a vertex v in G is the maximum distance from v to another vertex in G, *i.e.*, $ecc(v) = max\{d(v, u), u \in V\}$. The radius $r = r(G)$ of G is the smallest eccentricity in G, *i.e.*, $r = min\{ecc(v), v \in V\}$.

Theorem 6 [2,8]. *Let G be a connected graph on $n \geqslant 2$ vertices with index λ_1 and average distance $\overline{l}$. Then*

$$\lambda_1 + \overline{l} \leqslant n,$$

with equality if and only if G is the complete graph K_n.

Many of the conjectures of AGX Form 1 remain open (see Table 1). Before giving some examples, recalling some definitions is needed. A *matching* in a graph is a set of disjoint edges, and the maximum cardinality of a matching over all possible matchings in a graph G is *the matching number* of G and denoted by $\mu = \mu(G)$. A matching is *perfect* if it contains $n/2$ edges (so n is necessarily even), which is the largest possible value for μ. The vertex (resp. edge) connectivity ν (resp. κ) of G is the minimum number of vertices (resp. edges) whose removal disconnects G (or reduces it to a single vertex in the case of vertex connectivity).

Conjecture 7. *Let G be a connected graph on $n \geqslant 3$ vertices with index λ_1 and matching number μ. Then*

$$\lambda_1 - \mu \leqslant n - 1 - \lfloor n/2 \rfloor,$$

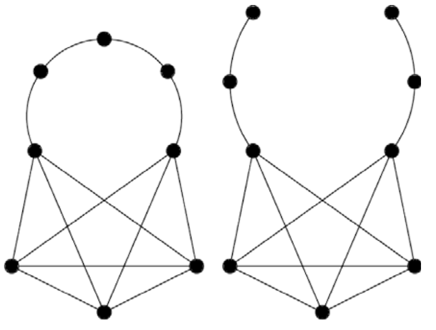

Fig. 5. An odd bag $Bag_{5,5}$ and a bug $Bug_{5,3,3}$.

with equality if and only if G is the complete graph K_n.

$$\lambda_1 + \mu \geqslant \sqrt{n-1} + 1 \quad \textit{and} \quad \frac{\lambda_1}{\mu} \leqslant \sqrt{n-1},$$

with equalities if and only if G is the star S_n.

Conjecture 8. *Let G be a connected graph on $n \geqslant 3$ vertices with index λ_1, vertex connectivity ν and edge connectivity κ. Then*

$$\lambda_1 - \nu \leqslant n - 3 + t; \quad \lambda_1 - \kappa \leqslant n - 3 + t; \quad \frac{\lambda_1}{\nu} \leqslant n - 2 + t; \quad \textit{and} \quad \frac{\lambda_1}{\nu} \leqslant n - 2 + t,$$

where t is such that $0 < t < 1$ and $t^3 + (2n-3)t^2 + (n^2 - 3n + 1)t - 1 = 0$. Equalities hold if and only if G is the kite $Ki_{n,n-1}$.

Among other results obtained as this automated comparison was done, two new families of extremal graphs related to the index were discovered. Indeed, the *bags* and *bugs* were studied for the first time, as extremal graphs related to the index, in [72]. A bag $Bag_{p,q}$ is a graph obtained from a complete graph K_p by replacing an edge uv with a path P_q. A bag is odd if q is odd, otherwise it is even. So, in $Bag_{p,q}$ the number of vertices is $n = p + q - 2$ and the number of edges is $m = \frac{p(p-1)}{2} + q - 2$. A bug Bug_{p,q_1,q_2} is a graph obtained from a complete graph K_p by deleting an edge uv and attaching paths P_{q_1} at u and P_{q_2} at v. A bug is balanced if $|q_1 - q_2| \leqslant 1$. So, in Bug_{p,q_1,q_2} the number of vertices is $n = p + q_1 + q_2 - 2$ and the number of edges is $m = \frac{p(p-1)}{2} + q_1 + q_2 - 3$. Fig. 5 gives examples of a bag and a bug. The main results proved in [72] are gathered in the following theorem. But first, recall that a matching in a graph is a set of disjoint edges, and the maximum cardinality of a matching over all possible matching in a graph G is the matching number of G and denoted by $\mu = \mu(G)$. A matching is perfect if it contains $n/2$ edges (so n is necessarily even), which is the largest possible value for μ.

Theorem 9

(1) *Among all connected graphs on n vertices with diameter D, the maximum index is attained by*

- *a complete graph K_n when $D = 1$, and*
- *a balanced bug $Bug_{n-D+2,\lfloor D/2 \rfloor,\lceil D/2 \rceil}$ when $D \geqslant 2$.*

(2) *Among all graphs on n vertices with radius r, the maximum index is attained by*

- *a complete graph K_n when $r = 1$,*
- *$K_n \setminus M$ for n even and $r = 2$, where M is a perfect matching,*

- $K_n \setminus (L \cup P_3)$ *for n odd and* $r = 2$, *where L is a matching with* $(n-3)/2$ *edges and* P_3 *the path on 3 vertices, and*
- *an odd bag* $Bag_{n-2r+3,2r-1}$ *when* $r \geqslant 3$.

Some statistics about the results of AGX Form 1 related to the index λ_1 are given in Table 1. The index λ_1 is compared to 19 other graph invariants. So there are 152 possible bounds.

Another more specific problem where AGX is involved is the characterization of extremal graphs for (minimum and maximum) values of λ_1 under color constraints. Actually, the problem is to find the extremal values of λ_1 when the numbers of *white* and *black* vertices in a tree are fixed. The results of this study are discussed in [38], and comprise the following theorem. First, recall that a *double star* DS_{Δ_1,Δ_2} is the tree obtained from two stars S_{Δ_1} and S_{Δ_2} by adding an edge between their central vertices. Also, a *comet* $Co_{n,\Delta}$ is the tree obtained from a star S_Δ and a path $P_{n-\Delta}$ by adding an edge between the central vertex of S_Δ and an endpoint of $P_{n-\Delta}$.

Theorem 10

(1) *The only tree with a black vertices and b white vertices that maximizes* λ_1 *is the double star* $S_{a,b}$.
(2) *The only tree with a black vertices and b white vertices, such that* $a = b + 2$ *and* $a + b \geqslant 6$, *that minimizes* λ_1 *is the comet* $C_{a+b,3}$.

In a sequel, using AGX, to find Nordhaus–Gaddum relations for the index λ_1, the following open conjecture was obtained.

Conjecture 11 [3]. *For any connected graph on* $n \geqslant 5$ *vertices we have*

$$\lambda_1(G) + \lambda_1(\overline{G}) \leqslant \frac{4}{3}n - \frac{5}{3} - \begin{cases} f_1(n) & \text{if} \quad n \bmod (3) = 1, \\ 0 & \text{if} \quad n \bmod (3) = 2, \\ f_2(n) & \text{if} \quad n \bmod (3) = 0, \end{cases}$$

where $f_1(n) = \frac{3n-2-\sqrt{9n^2-12n+12}}{6}$ *and* $f_2(n) = \frac{3n-1-\sqrt{9n^2-6n+9}}{6}$. *The equality holds if and only if G the complete split graph with an independent set on* $\left\lfloor \frac{n}{3} \right\rfloor$ *vertices, and also on* $\lceil \frac{n}{3} \rceil$ *vertices if* $n \bmod (3) = 2$.

2.2. Second largest eigenvalue

The study of the second largest eigenvalue (of the adjacency matrix) of a graph attracted an important number of researchers. Actually, the characterization of the graphs for which the second largest eigenvalue belongs to a specified interval of values is the most important field studied during the last four decades (see [36,121] for references). The graphs whose second largest eigenvalue is less than or equal to $\frac{1}{3}$ are characterized in [17] as follows.

Theorem 12. *For a graph G of order n without isolated vertices,* $0 < \lambda_2(G) < 1/3$ *if and only if* $G = \overline{K}_{n-3} \vee (K_1 \cup K_2)$, *the graph obtained by joining each vertex of* $\overline{K}_{n-3}$ *(the complementary of* K_{n-3}*) to each vertex of* $K_1 \cup K_2$ *(see Fig. 6 for* $K_6 \vee (K_1 \cup K_2)$*).*

In the same paper, the problem of characterizing graphs G with $\frac{1}{3} < \lambda_2(G) < \left(\sqrt{5}-1\right)/2$ was posed. It was discussed in several papers such as [36,108,109]. In these papers, a graph G is said to have the σ-property (or to be a σ-graph) if its second largest eigenvalue does not exceed $\sigma = \left(\sqrt{5}-1\right)/2$. The σ-graphs are characterized using forbidden subgraphs in the following theorem [109].

Theorem 13. *If H is a minimal forbidden induced subgraph for the* σ*-property, then one of the following statements is true.*

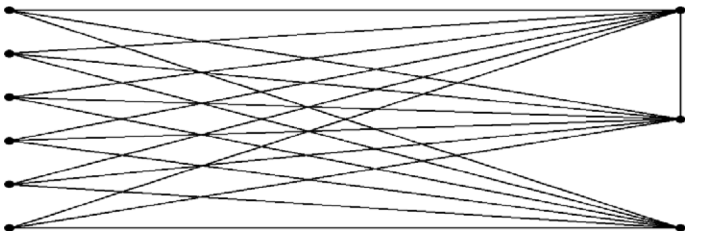

Fig. 6. The graph $\overline{K_6} \vee (K_1 \cup K_2)$.

Fig. 7. Some forbidden graphs for σ-property.

(1) *H is one of the graphs* $2K_2, F_1, F_2, F_3$ *or* F_4 (*see Fig.* 7).
(2) *H belongs to the family* $\mathcal{C}$, *recursively defined by:*

(a) *the empty graph belongs to* $\mathcal{C}$;
(b) *if* $G \in \mathcal{C}$, *then* $G \cup pK_1 \in \mathcal{C}, p \in \mathbb{N}$;
(c) *if* $G_1, G_2 \in \mathcal{C}$, *then* $G_1 \vee G_2 \in \mathcal{C}$;
(d) *any graph from* $\mathcal{C}$ *can be obtained only using the above rules.*

Many other ranges for $\lambda_2(G)$ were explored such as characterizing graphs with $\lambda_2(G)$ at most $\sqrt{2}-1$ [102] or less than 1 [119].

The following theorem proved in [54] was first obtained by the use of the Graffiti program.

Theorem 14. *Let* $G \ncong K_2$ *be a graph with m edges and clique number* ω. *Then* $|\lambda_2| \leqslant m/\omega$.

The bound in the above theorem is not tight, so it is natural to search for a tight upper bound on $|\lambda_2|$ in terms of m and ω. This was done using AGX and the following conjecture was obtained.

Conjecture 15. *Let G be a connected graph on n vertices with clique number* ω *and second largest eigenvalue* λ_2. *Then*

- *if n is odd,* $|\lambda_2| \cdot \omega \leqslant m - 2$ *with equality if and only if G is composed of* $K_{\frac{n+1}{2}}$ *and* $K_{\frac{n-1}{2}}$ *linked by an edge or of* $K_{\frac{n-1}{2}}$ *and* $K_{\frac{n-1}{2}}$ *linked by a path;*
- *if n is even,* $|\lambda_2| \cdot \omega - m$ *is maximum if and only if G is composed of two copies of* $K_{\frac{n}{2}}$ *linked by an edge.*

The next conjecture is due to Gernert (see <http://www.sgt.pep.ufrj.br/>) who proved it for all regular graphs and has verified it for several other classes of graphs, such as planar, complete multipartite and triangle-free graphs (see, also [47]).

Conjecture 16. *If G is a graph of order n and* λ_1 *and* λ_2 *are the two largest eigenvalues of G, then* $\lambda_1 + \lambda_2 \leqslant n$.

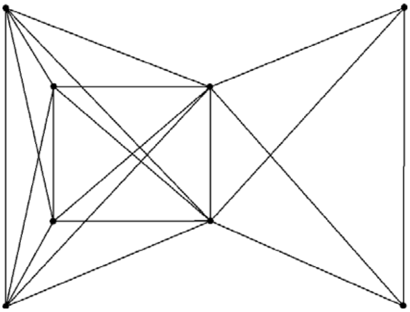

Fig. 8. The graph $G(8,4,2)$.

This conjecture was refuted by Nikiforov [47,98]. It was independently, but later, studied using AGX. After refuting it again, a new conjecture was found.

Consider the graph H on $n \geqslant 5$ vertices composed of the complete bipartite graph $K_{p,q}$ and $n-p-q$ isolated vertices. Let $G(n,p,q)$ denote the complement of H (see Fig. 8 for $G(8,4,2)$).

Conjecture 17. *Let $G=(V,E)$ be a connected graph on $n \geqslant 5$ vertices with largest and second largest eigenvalues λ_1 and λ_2 respectively. Then*

$$\lambda_1 + \lambda_2 \leqslant \lambda_1(G(n,p,q)) + \lambda_2(G(n,p,q))$$

where

$$p = \begin{cases} 2\left\lfloor \frac{n}{7} \right\rfloor & \text{if } n = 0,1 \, mod(7), \\ 2\left\lfloor \frac{n}{7} \right\rfloor + 1 & \text{if } n = 2,3,4 \, mod(7), \\ 2\left\lfloor \frac{n}{7} \right\rfloor + 2 & \text{if } n = 5,6 \, mod(7) \end{cases} \quad and \quad q = \begin{cases} 2\left\lfloor \frac{n}{7} \right\rfloor & \text{if } n = 0,1,2 \, mod(7), \\ 2\left\lfloor \frac{n}{7} \right\rfloor + 1 & \text{if } n = 3,4,5 \, mod(7), \\ 2\left\lfloor \frac{n}{7} \right\rfloor + 2 & \text{if } n = 6 \, mod(7). \end{cases}$$

Moreover $\lambda_1(G(n,p,q)) + \lambda_2(G(n,p,q)) \leqslant 8n/7 - 2$ with equality if and only if $n = 0 \, mod(7)$.

The part $n = 0 \, mod(7)$ of the above conjecture was also conjectured by the authors of [47]. They did not consider the case $n \neq 0 \, mod(7)$ in their conjecture.

2.3. Smallest eigenvalue

The smallest eigenvalue λ_n of a graph is the third eigenvalue to attract the interest of many researchers, after the largest and second largest eigenvalues. As for λ_1 and λ_2, the computer was used to derive conjectures about λ_n. Indeed, the following list of results are first conjectured using the program Graffiti and then proved by hand in [54]. Recall that the *Randić index* [104] of a graph G is defined by

$$Ra(G) = \sum_{uv \in E} \frac{1}{\sqrt{d(u) \cdot d(v)}}.$$

Recall that the complementary graph $\overline{G}$ of a graph $G=(V,E)$ (or the complement of G, for short) has the same vertex set V as G and an edge joining vertices u and v if and only if there is no such edge in G.

Theorem 18. *Let G be a connected graph on m edges with Randić index Ra and matching number μ. Let $\bar{\mu}$ denote the matching number of the complement $\overline{G}$ of G. Then*

(1) $|\lambda_n| \leqslant Ra$;
(2) $|\lambda_n| \leqslant \sqrt{m}$;
(3) $|\lambda_n| \leqslant \mu + \bar{\mu}$.

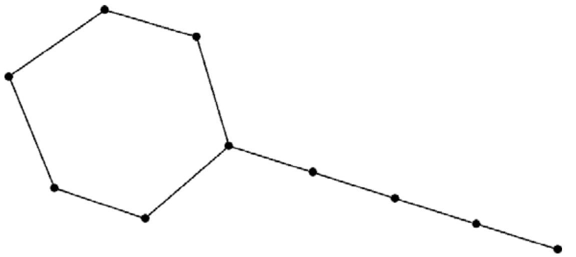

Fig. 9. The lollipop $Lol_{10,6}$.

2.4. Negative and positive eigenvalues and energy

The following theorem, first conjectured using Graffiti, gives an upper bound on the number of positive eigenvalues of a graph in terms of the matching number of a graph G and its complement $\overline{G}$.

Theorem 19 [54]. *For any graph G with matching number μ and p^+ distinct positive eigenvalues, $p^+ \leqslant \mu + \bar{\mu}$, where $\bar{\mu}$ is the matching number of the complement $\overline{G}$ of G.*

The next two theorems are stated for positive eigenvalues, but since the sum of all eigenvalues of the adjacency matrix is zero, they can be stated also in terms of negative eigenvalues.

Theorem 20 [54]. *Let G be a graph with matching number μ and eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. Let q be the integer such that $\lambda_q > 0$ and $\lambda_{q+1} \leqslant 0$. Then $\mu \leqslant \lambda_1 + \lambda_2 + \cdots + \lambda_q$.*

The following theorem conjectured by Graffiti is proved in [49], the second paper devoted to list Graffiti's conjectures.

Theorem 21. *Let G be a graph with radius r and eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. Let q be the integer such that $\lambda_q > 0$ and $\lambda_{q+1} \leqslant 0$. Then $r \leqslant \lambda_1 + \lambda_2 + \cdots + \lambda_q$.*

The *energy* $E(G)$ of a graph G is defined as the sum of the absolute values of its eigenvalues, *i.e.*

$$E(G) = \sum_{i=1}^{n} |\lambda_i(G)| = 2 \sum_{\lambda_i > 0} \lambda_i = 2 \sum_{\lambda_i < 0} |\lambda_i|.$$

A lollipop $Lol_{n,g}$, with $n \geqslant g \geqslant 3$, is a graph obtained from a cycle C_g and a path P_{n-g} by adding an edge between a vertex from the cycle and an endpoint from the path (see Fig. 9 for $Lol_{10,6}$). $Lol_{n,n-1}$ is called the short lollipop while $Lol_{n,3}$ is the long lollipop and $Lol_{n,n}$ is the cycle C_n.

In order to find lower and upper bounds on the energy, Caporossi et al. [19] used the AGX system. They found the following conjectures afterwards proved by hand.

Theorem 22. *Let G be a simple graph on n vertices and m edges with energy E. Then*

(1) $E \geqslant \frac{4m}{n}$;
(2) $E \geqslant 2\sqrt{m}$ *with equality if and only if G is a complete bipartite graph plus possibly some isolated vertices*;
(3) *if G is connected, $E \geqslant 2\sqrt{n-1}$ with equality if and only if G is the star S_n*;
(4) $E \leqslant 2m$ *with equality if and only if G is composed of disjoint edges and possibly isolated vertices*.

In this study, the particular case of unicyclic graphs was considered. Some unicyclic graphs that maximize the energy are given in Fig. 10. The following conjecture was stated.

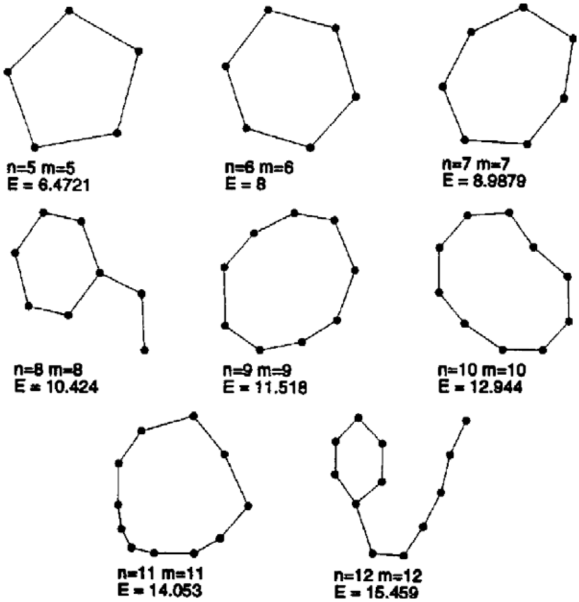

Fig. 10. Unicyclic graphs with largest energy for $n = 5 - 12$.

Conjecture 23. *Among unicyclic graphs on n vertices the cycle C_n has maximal energy if $n \leqslant 7$ and $n = 9, 10, 11, 13$ and 15. For all other values of n the unicyclic graph with maximum energy is the lollipop $Lol_{n,6}$.*

A weaker form of this conjecture is proved in [75] (in which unicyclic graphs that maximize the energy are discussed), namely the following theorem.

Theorem 24. *Let G be a connected, unicyclic and bipartite graph on $n \geqslant 7$ vertices and $G \ncong C_n$. Then $E(G) \leqslant E(Lol_{n,6})$.*

In [66], Gutman conjectured that among all graphs on n vertices, the complete graph K_n has the greatest energy $E(K_n) = 2n - 2$. By the use of the computer, namely the system GRAPH, Gutman and Cvetković [31] did find the smallest graph G on $n = 8$ vertices with $E(G) > 2n - 2$. A graph G on n vertices with energy $E(G) > 2n - 2$, is called a *hyperenergetic graph* [74]. After that infinite families of hyperenergetic graphs were defined. A *line graph* $L(G)$ of the graph $G = (V, E)$ is the graph where the set of vertices is the set of edges E of G and where two vertices (of $L(G)$) are adjacent if and only if their corresponding edges in G are incident to the same vertex of G. Walikar et al. [118] proved that the line graph $L(K_p)$ is hyperenergetic for all $p \geqslant 5$. Gutman [67] gave another general method for constructing hyperenergetic graphs by deleting few edges from complete graphs K_n. This method furnishes hyperenergetic graphs for all $n \geqslant 9$.

2.5. Integral graphs

A graph whose spectrum consists entirely of integers is called an *integral graph*. *Which graphs have integral spectra?* This question was first posed by Harary and Schwenk in [73]. Despite the facts that their number is infinite and their existence among a huge number of families of graphs, the integral graphs are rare and difficult to find. For instance, among the class of cubic (regular of degree 3) graphs, there are exactly 13 integral graphs [16]. For a survey and references about integral graphs see [9].

As finding integral graph is a difficult task, the computer was involved. Indeed, for instance it was used to find all 4-regular bipartite graphs on up to 24 vertices [117]. These investigations yield to a

Table 2
The number of integral graphs among 4-regular bipartite graphs.

Order	4-Regular bipartite graphs	Integral graphs	Time (s)
8	1	1	< 1
10	1	1	< 1
12	4	2	< 1
14	16	1	< 1
16	193	3	< 1
18	3528	7	11
20	121,785	11	499
24	317,579,563	21	10,441,176

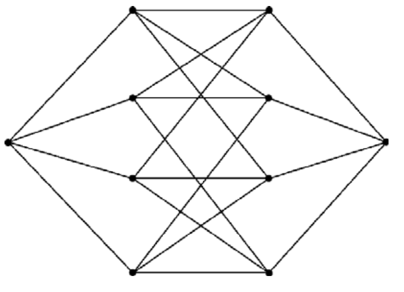

Fig. 11. Integral graph with a spectrum $\left(4, 1^{(4)}, -1^{(4)}, -4\right)$.

total of 47 integral graphs (note that there are 317,579,563 4-regular bipartite graphs with 24 vertices). Namely, three computer programs were used: **genbg** (a component of the package nauty by Brendan D. McKay, available at http://cs.anu.edu.au/~bdm/nauty) is used to generate all the graphs on up to 24 vertices; **integrality** calculates (using the **eigens** procedure written by S. Moshier and available at http://www.koders.com/) the spectrum of each graph and selects the integral ones; **neato** (from the package **GraphViz**, available at http://www.graphviz.org) is used to draw the graphs selected by **integrality**. Table 2 from [117], which contains the number of 4-regular connected graphs, the number of integral graphs (one of which is given in Fig. 11) and the computation time for each order up to 24, gives an idea of the rarity of and the difficulty of finding integral graphs. Note that it was previously known that there are no 4-regular bipartite integral graphs on 22 vertices.

3. Laplacian

The *Laplacian* matrix (or Laplacian, for short) of a graph G is defined by $L = Diag - A$, where $Diag$ is the diagonal matrix which entries are the degrees of the vertices of G, and A is the adjacency matrix of G. Let $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{n-1} \geqslant \mu_n = 0$ denote the eigenvalues of L. They are usually called the Laplacian eigenvalues of G. Note that $\mu_n = 0$ for any graph.

3.1. The algebraic connectivity

Among all eigenvalues of the Laplacian of a graph, the most studied is the second smallest, called the algebraic connectivity of a graph [55]. Its importance is due to the fact that it is a good parameter to measure how well a graph is connected. For example, it is well known that a graph is connected if and only if $a \neq 0$. Recently, the algebraic connectivity has been the subject of many publications, see [25,55,61,64,87–89] for surveys and books and in particular [39], which mentions [62,63,79,83,85,97,105] for application on trees; [11,51,52,56,57,64,92,93,96] for applications on more specific problems in graph theory; [10,30,56,58,77,82,92,93] for applications on combinatorial optimization problems; [46,107] for the study of the asymptotic behavior of the algebraic connectivity for random graphs. Besides, the algebraic connectivity is of relevance to various fields of mathematics: the theory of

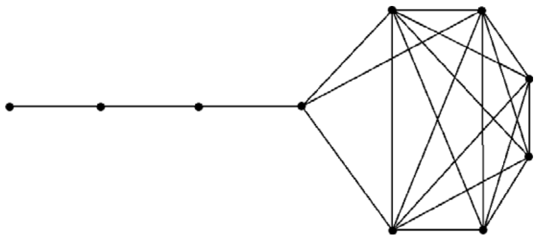

Fig. 12. A Soltés graph.

elasticity [107]; the correspondence between continuous and discrete mathematics [23]; bandwidth-type problems [92]; convex optimization [60]. The Fiedler vectors, *i.e.*, the eigenvectors corresponding to the algebraic connectivity, have also received a lot of attention recently, see [51,79,80,90] for general graphs and [62,63,79] for trees. More recently, the limit points of Laplacian spectra, and so of the algebraic connectivity, have been a subject of interest [65,76,100]. Finally, during the last decade, the characterization of the extremal graphs related to extremal values (minima and maxima) of invariants seems to place a great emphasis on graph theory research. This includes the extremal graphs related to the algebraic connectivity [10,53,78,80].

In this section, we only deal with some of the results about the algebraic connectivity obtained using the computer. The first such results obtained using AGX are discussed in [10], where one can find the following theorem and open conjecture.

Theorem 25. *If G is a connected graph with m edges such that $G \not\cong K_n$, then $a(G) \leqslant \left\lfloor -1 + \sqrt{1+2m} \right\rfloor$, and this bound is sharp for all $m \geqslant 2$.*

A *path-complete graph*, also called a *Soltés graph*, $PK_{n,m}$ is the graph on n vertices and m edges obtained from a clique and a path by adding at least one edge between the clique and an endpoint from the path (see Fig. 12 for an example). Note that for fixed n and m there exists exactly one $PK_{n,m}$.

Conjecture 26. *The connected graphs $G \not\cong K_n$ with minimum algebraic connectivity are path-complete graphs.*

Among the invariants involved when a systematic automated comparison of graph invariants [2] was done, one can find the algebraic connectivity. One of the results is the following theorem.

Theorem 27 [2,7]. *If G is a connected graph on n vertices with average distance $\bar{l}$. then $a \cdot \bar{l} \leqslant n$ and $a + \bar{l} \leqslant n + 1$ with equality in both cases if and only if G is the complete graph K_n.*

Note that the above bound on the product was also conjectured by the computer program Graffiti (Conjecture 128 [50]). As a corollary of the above theorem we have the following bounds which were themselves first conjectured by the AGX system. But before the statement of the corollary we need these definitions. The transmission $t(u)$ a vertex u in a connected graph G is the sum of distances from u to all other vertices, *i.e.*, $t(u) = \sum_{v \in V} d(u, v)$. It is said to be normalized and denoted by $\tilde{t}(v)$ if divided by $n - 1$, where n is the number of vertices in G, *i.e.*, $\tilde{t}(v) = t(v)/(n-1)$. The proximity $\pi(G)$ of a connected graph G is the minimum normalized transmission in G while the maximum is the remoteness $\rho(G)$, *i.e.*, $\pi = \pi(G) = min\{\tilde{t}(v), v \in V\}$ and $\rho = \rho(G) = max\{\tilde{t}(v), v \in V\}$.

Corollary 28. *If G is a connected graph on n vertices with proximity π, then $a \cdot \pi \leqslant n$ and $a + \pi \leqslant n + 1$ with equality in both cases if and only if G is the complete graph K_n.*

Fig. 13. A graph composed of 2 triangles linked by a path.

We next give a list of conjectures of AGX Form 1 obtained using AGX [2,5].

Conjecture 29. *Let G be a connected graph on $n \geqslant 5$ vertices with algebraic connectivity a and average distance $\bar{l}$. Then*

- $a + \bar{l}$ *is minimum for the kite* $Ki_{n,n-2}$;
- $a \cdot \bar{l}$ *is minimum for the graph composed of* 2 *triangles linked by a path (see Fig.* 13 *for an example of such a graph).*

Conjecture 30. *Let G be a connected graph on n vertices with proximity π and algebraic connectivity a. Then*

$$\pi \cdot a \geqslant \begin{cases} \frac{3n+1}{2}\,\frac{n-1}{n}\left(1 - \cos\frac{\pi}{n}\right) & \text{if } n \text{ is odd,} \\ \frac{3n-2}{2}\left(1 - \cos\frac{\pi}{n}\right) & \text{if } n \text{ is even,} \end{cases}$$

with equality if and only if G is the path P_n.

The *girth* $g = g(G)$ of a graph G on n vertices with at least n edges is the length of the smallest cycle in G.

Conjecture 31. *Let G be a connected graph on n vertices with girth g and algebraic connectivity a. Then*

- $a + g$ *and* $a \cdot g$ *are minimum for the kite* $Ki_{n,3}$;
- a/g *is minimum for the lollipop* $Lol_{n,\lfloor n/2 \rfloor}$.

Conjecture 32. *Let G be a connected graph on n vertices with matching number μ and algebraic connectivity a. Then $a \cdot \mu \geqslant 1$ with equality if and only if G is the star S_n.*

Conjecture 33. *Let G be a connected graph on n vertices with index λ_1 and algebraic connectivity a. Then*

- $a - \lambda_1 \geqslant 3 - n - t$, *where* $0 < t < 1$ *and* $t^3 + (2n-3)t^2 + (n^2 - 3n + 1)t - 1 = 0$, *with equality if and only if G is the kite* $Ki_{n,n-1}$;
- a/λ_1 *is minimum for the kite* $Ki_{n,\lfloor \frac{n}{2} \rfloor}$.

As in the case of the index, we finish this subsection by giving in Table 3 some statistics about AGX Form 1 results related to the algebraic connectivity.

3.2. The largest Laplacian eigenvalue

Besides the algebraic connectivity, the largest Laplacian eigenvalue μ_1 is the invariant that interested the graph theorists. Finding an upper bound to μ_1 is the most studied problem.

One of the problems studied using newGRAPH is finding upper bounds on the largest eigenvalue of the Laplacian of a graph. Recall that the *Laplacian* of a graph G is defined by $L = D - A$, where D is the diagonal matrix which entries are the degrees of the vertices of G, and A is the adjacency matrix of G. The spectral graph theorists are increasingly interested in the largest eigenvalue μ_1 of L. This interest

Table 3
Statistics for AGX Form 1 conjectures about a.

Results type	Number of results	%
Known results	5	3.29
Automated proof	68	44.74
Proved by hand	33	21.71
Open (complete) conjectures	22	14.47
Structural open conjectures	18	11.84
Refuted conjectures	0	0.00
No result	6	3.95

is mainly due to the numerous applications of μ_1: (i) it is used in theoretical chemistry to determine the first ionization potential of alkanes [68]; (ii) in combinatorial optimization, μ_1 provides an upper bound on the size of the maximum cut in graphs [43–45,95,103]; (iii) it also provides a lower bound on the edge-forwarding index, in communication networks [112]. Other applications of μ_1 are discussed in [94]. Using a computer program, Brankov et al. [12] generated known and new upper bounds on the largest Laplacian eigenvalue μ_1. Among the known bounds, one can find

$$\mu_1 \leqslant \max_{ij \in E} d_i + d_j \quad [1],$$

$$\mu_1 \leqslant \max_{ij \in E} \frac{d_i(d_i + m_i) + d_j(d_j + m_j)}{d_i + d_j} \quad [81],$$

$$\mu_1 \leqslant \max_{ij \in E} \sqrt{d_i(d_i + m_i) + d_j(d_j + m_j)} \quad [120],$$

$$\mu_1 \leqslant \max_{ij \in E} 2 + \sqrt{d_i(d_i + m_i - 4) + d_j(d_j + m_j - 4) + 4} \quad [120],$$

$$\mu_1 \leqslant \max_{ij \in E} \frac{d_i + d_j + \sqrt{(d_i - d_j)^2 + 4m_i m_j}}{2} \quad [40],$$

where d_i denotes the degree of a vertex $i \in V$ and m_i denotes the average of the degrees of the neighbors of the vertex i.

A list of 76 upper bounds on μ_1 conjectured using an *unnamed* specialized computer program is given in [12], of which the following ones:

$$\max_{i \in V} m_i + d_i,$$

$$\max_{i \in V} \sqrt{d_i(m_i + 3d_i)},$$

$$\max_{i \in V} \sqrt{m_i(d_i + 3m_i)},$$

$$\max_{ij \in E} 2 + \sqrt{2(d_i^2 + d_j^2) - 4(d_i + d_j) + 4},$$

$$\max_{ij \in E} 2 + \sqrt{2(d_i^2 + d_j^2) - 4(m_i + m_j) + 4},$$

$$\max_{ij \in E} 2 + \sqrt{(m_i - m_j)^2 + 4d_i d_j - 4(m_i + m_j) + 4}.$$

The first of these bounds is known [86].

Two types of bounds are studied. In one case, the maximum is taken over the set of vertices, *i.e.*, bounds of the form

$$\mu_1 \leqslant \max_{i \in V} f(d_i, m_i). \tag{2}$$

In the other case, the maximum is taken over the set of edges, *i.e.*, bounds of the form

$$\mu_1 \leqslant \max_{ij \in E} f(d_i, d_j, m_i, m_j). \tag{3}$$

The process that led to the above upper bounds on μ_1 is composed of 3 steps.

(i) *Generating* bounds is the first step. Its principle is based on the observation that all the known bounds on μ_1 given above are reached for regular bipartite graphs, in which case $d_i = m_i = x$ for all $i \in V$ and $\mu_1 = 2x$. Thus, to be a candidate for bounding μ_1, any expression must first satisfy $f(x, x) = 2x$ for the form (2) and $f(x, x, x, x) = 2x$ for the form (3). Therefore, the first step consists of performing algebraic operations that preserve these conditions, on a set of known bounds. To illustrate, in the case of bounds of the form (2), starting from two known bounds f_1 and f_2, we can perform one or more of the following transformations:

(T1) $f' = \dfrac{f_1 + f_2}{2}$;

(T2) $cf' = kf_1 + (c - k)f_2$, where $c \in \mathbb{N}$ and $1 \leqslant k < c$;

(T3) $f' = \dfrac{xf_1}{x}$;

(T4) $f' = \sqrt{f_1 \cdot f_2}$.

For instance,

- starting from the expression $2x$;
- apply (T4) to get the expression $\sqrt{2x \cdot 2x}$;
- apply (T1) to get the expression $\frac{2x+\sqrt{2x \cdot 2x}}{2}$;
- replace the first and second occurrences of x by d_i and the last occurrence of x by m_i, to reproduce the following bound proved in [120]

$$\mu_1 \leqslant \max_{v_i \in V} d_i + \sqrt{d_i m_i}.$$

(ii) In the second step, called *testing* step, the generated bounds are tested on the set of all connected graphs on up to nine vertices. There are more than 273,000 such graphs. They are generated using McKay's computer program nauty. Also some of special graphs, known to have well suited values of μ_1, d_i and m_i, are added to the test set of graphs. Among these graphs, one can find stars S_n and *windmills* W_{2k+1}. A windmill W_{2k+1} is the graph obtained from k copies of K_2 by adding a central vertex adjacent to all other vertices.

(iii) Finally, in the *covering and statistics* step, the dominance among the bounds that pass the testing step is checked and only the bounds that are not dominated are retained. A statistic is associated to the retained bounds in order to illustrate their relative importance.

4. Signless Laplacian

The *signless Laplacian* of a graph G is defined by $Q = D + A$, where D is the diagonal matrix which entries are the degrees of the vertices of G, and A is the adjacency matrix of G. Let $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$ denote the eigenvalues of Q. They are usually called the signless Laplacian eigenvalues of G. AGX was used to study the signless Laplacian of a connected graph, and a series of 30 conjectures were obtained. These conjectures are listed and some of them are proved in [34]. First, the following theorem gives a characterization of the complete graph using the number of distinct signless Laplacian eigenvalues or the multiplicity of the second largest signless Laplacian eigenvalue.

Theorem 34. *Let G be a connected graph on $n \geqslant 2$ vertices. The following statements are equivalent.*

- *The number of distinct signless Laplacian eigenvalues of G is* $e(G) = 2$.
- *The multiplicity of the second largest signless Laplacian eigenvalue of G is* $m(q_2) = n - 1$.
- *G is the complete graph* K_n.

Some of the proved conjectures related to the largest signless Laplacian eigenvalue are gathered in the following theorem.

Theorem 35. *Let G be a connected graph on* $n \geqslant 4$ *vertices with largest signless eigenvalue* q_1 *and maximum degree* Δ. *Then*

- $2 + 2\cos\frac{\pi}{n} \leqslant q_1 \leqslant 2n - 2$ *with equality if and only if G is* P_n *for the lower bound and if and only if G is* K_n *for the upper bound;*
- *if G is a tree,* $2 + 2\cos\frac{\pi}{n} \leqslant q_1 \leqslant n$ *with equality if and only if G is* P_n *for the lower bound and if and only if G is* S_n *for the upper bound;*
- *if G is unicyclic,* $4 \leqslant q_1 \leqslant q_1(S_n^+)$ *with equality if and only if G is* C_n *for the lower bound and if and only if G is* S_n^+ *for the upper bound;*
- $q_1 \geqslant \Delta + 1$ *with equality if and only if G is* S_n.

The following conjecture gatheres questions about the index of the signless Laplacian, which remain open.

Conjecture 36. *If G is a connected graph on* $n \geqslant 4$ *vertices with largest signless Laplacian eigenvalue* q_1, *largest Laplacian eigenvalue* μ_1, *index* λ_1 *and average degree* $\bar{d}$, *then*

- $q_1 - 2\bar{d} \leqslant n - 4 + 4/n$ *with equality if and only if G is* S_n;
- $q_1 - \bar{d} \leqslant n - 1$ *with equality if and only if G is* K_n;
- $q_1 - \lambda_1 - \bar{d} \leqslant n - 2 + 2/n - \sqrt{n-1}$ *with equality if and only if G is* S_n;
- $\mu_1 + \lambda_1 - q_1 \leqslant \sqrt{\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil}$ *with equality if and only if G is* $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$;
- $q_1 - \mu_1 \leqslant n - 2$ *with equality if and only if G is* K_n;
- $q_1 - 2\lambda_1 \leqslant n - 2\sqrt{n-1}$ *with equality if and only if G is* S_n.

The second largest signless Laplacian eigenvalue q_2 was also considered in the same study [34]. Almost all AGX conjectures about q_2 remain open. Examples are gathered below. Note that there are some border effects, for instance in the case of the upper bound on $q_2 - \delta$ we need to have $n \geqslant 7$.

Conjecture 37. *If G is a connected graph* $n \geqslant 4$ *vertices with second largest signless Laplacian eigenvalue* q_2, *index* λ_1, *algebraic connectivity a, and minimum, average and maximum degree* δ, $\bar{d}$ *and* Δ *respectively, then*

- $q_2 - \bar{d} \geqslant -1$ *with equality if and only if G is* K_n;
- $q_2 - \bar{d} \leqslant n - 6 + 8/n$ *with equality if and only if G is the complete bipartite graph* $K_{n-2,2}$;
- $q_2 - \delta \geqslant -1$ *with equality if and only if G is* K_n;
- $q_2 - \delta \leqslant n - 3$ *with equality if and only if G is the kite* $Ki_{n,n-1}$;
- $\Delta - q_2 \leqslant n - 2$ *with equality if and only if G is* S_n;
- $q_2 - \lambda_1 \geqslant 1 - \sqrt{n-1}$ *with equality if and only if G is* S_n;
- $q_2 - \lambda_1 \leqslant n - 2 - \sqrt{2n-4}$ *with equality if and only if G is* $K_{n-2,2}$;
- $q_2 - a \geqslant -2$ *with equality if and only if G is* K_n;
- *if G is not isomorphic to* K_n, *then* $q_2 - a \geqslant 0$.

The smallest signless Laplacian eigenvalue q_n was also considered, but only three conjectures were obtained, one of which is proved and two remain open. All three are given below, but first we need to recall a definition. A *complete split graph* $SK_{n,\alpha}$ is the graph obtain from a clique on $n - \alpha$ vertices and α isolated vertices by adding all possible edges from each of the isolated vertices to all vertices of the clique (see Fig. 14 for $SK_{10,6}$).

Theorem 38 [22]. *If G is a connected and not a bipartite graph, then* $q_n \geqslant q_n(Lol_{n,3})$ *with equality if and only if G is* $Lol_{n,3}$.

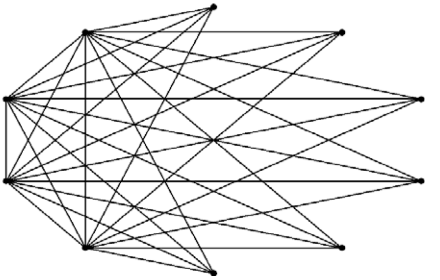

Fig. 14. The complete split graph $SK_{10,6}$.

Conjecture 39. *Over all connected graphs on $n \geqslant 6$ vertices, $q_1 - q_n$ is minimum for the path P_n and for the odd cycle C_n, and is maximum for the kite $Ki_{n,n-1}$.*

Conjecture 40. *For any connected graph G on $n \geqslant 4$ vertices with independence number α, $q_1 + q_n + 2\alpha \leqslant 3n - 2$ with equality if and only if G is the complete split graph $SK_{n,\alpha}$.*

5. The eigenvalues of the distance matrix

The distance matrix $\mathcal{D}$ of a connected graph G is defined by its ij entry as the distance between the two vertices v_i and v_j (according to a given labeling of the vertices). The only computer program that dealt with the eigenvalues of the distance matrix (the distance eigenvalues) of a graph is Graffiti [50]. Some conjectures were generated among which the following.

Theorem 41.

(1) The diameter of a connected graph is not more than the absolute value of its largest negative distance eigenvalue.
(2) The diameter of a connected graph is not more than the number of its negative distance eigenvalues.

Conjecture 42. *Let G be a triangle-free graph on n vertices with m edges, independence number α. If $p^-(\mathcal{D})$ denotes the number of negative distance eigenvalues of G then $m/\alpha \leqslant p_-(\mathcal{D})$ and $m/\alpha \leqslant n - p_-(\mathcal{D})$.*

As far as we know this conjecture is open.

Appendix

In Tables 4 and 5, we summarize the results from the automated comparison of graph invariants [2]. In the first and last columns, we point out the status (S) of the result with O for open, P for proved, K for known (before the comparison), T for trivial (when deduced immediately from the bounds of λ_1 and I), R for refuted and N when no result was obtained. The second and the sixth columns represent the extremal graphs for the lower and upper bounds respectively, while in the third and fifth columns are given the upper and lower bounds respectively. The fourth column is dedicated to the expression $\lambda_1 \oplus I$ where $\oplus$ is one of the operations $-, +, /, \times$ and I the invariant to which λ_1 is compared.

In Table 6, we summarize the Graffiti conjectures concerning graph spectra, according to the Written on the Wall file [50]. The following notation (not defined above) are used.

If *Vec* is a vector, $\min(Vec)$, $Mn(Vec)$ and $\max(Vec)$ denote the minimum, average and maximum of the entries of *Vec*. The *range* $Rg(Vec)$ of the vector *Vec* is the number of its distinct entries. The *scope* $Sp(Vec)$ is the difference between its maximum and minimum values, *i.e.*, $Sp(Vec) = \max(Vec) - \min(Vec)$. The *mode* $Md(Vec)$ of the vector *Vec* is the component of which that occurs most often. The

Table 4
AGX Form 1 conjectures about the index λ_1.

S	G for l_n	l_n	$\lambda_1 \oplus I$	u_n	G for u_n	S
P	S_n	$\sqrt{n-1}-n+1$	$\lambda_1 - \Delta$	0	Regular	K
T	P_n	$2+2\cos\frac{\pi}{n+1}$	$\lambda_1 + \Delta$	$2n-2$	K_n	T
P	S_n	$\sqrt{n-1}/(n+1)$	λ_1/Δ	1	Regular	K
T	P_n	$4\cos\frac{\pi}{n+1}$	$\lambda_1 \cdot \Delta$	$(n-1)^2$	K_n	T
K	Regular	0	$\lambda_1 - \bar{d}$		Pineapples	O
T	P_n	$2-\frac{2}{n}+2\cos\frac{\pi}{n+1}$	$\lambda_1 + \bar{d}$	$2n-2$	K_n	T
K	Regular	1	$\lambda_1/\bar{d}$	$n/(2\sqrt{n-1})$	S_n	P
T	P_n	$\left(4-\frac{4}{n}\right)\cdot\cos\frac{\pi}{n+1}$	$\lambda_1 \cdot \bar{d}$	$(n-1)^2$	K_n	T
K	Regular	0	$\lambda_1 - \delta$	$n-3+t$[a]	$Ki_{n,n-1}$	P
T	P_n	$1+2\cos\frac{\pi}{n+1}$	$\lambda_1 + \delta$	$2n-2$	K_n	T
K	Regular	1	λ_1/δ	$n-2+t$[a]	$Ki_{n,n-1}$	P
T	P_n	$2\cos\frac{\pi}{n+1}$	$\lambda_1 \cdot \delta$	$(n-1)^2$	K_n	T
T	P_n	$2\cos\frac{\pi}{n+1}-\frac{n+1}{3}$	$\lambda_1 - \bar{l}$	$n-2$	K_n	T
			$\lambda_1 + \bar{l}$	n	K_n	P
T	P_n	$\frac{6}{n+1}\cos\frac{\pi}{n+1}$	$\lambda_1/\bar{l}$	$n-1$	K_n	T
N			$\lambda_1 \cdot \bar{l}$	$\frac{(n-3+\sqrt{n^2+2n-7})}{2}$	$K_n - e$	R
T	P_n	$2\cos\frac{\pi}{n+1}-n+1$	$\lambda_1 - D$	$n-2$	K_n	T
R	S_n	$2+\sqrt{n-1}$	$\lambda_1 + D$	$n-1+2\cos\frac{\pi}{n+1}$	P_n	O
T	P_n	$\frac{2}{n-1}\cos\frac{\pi}{n+1}$	λ_1/D	$n-1$	K_n	T
R	S_n	$2\sqrt{n-1}$	$\lambda_1 \cdot D$		Bug_{p,q_1,q_2}[b]	O
T	P_n	$2\cos\frac{\pi}{n+1}-\left\lfloor\frac{n}{2}\right\rfloor$	$\lambda_1 - r$	$n-2$	K_n	T
N			$\lambda_1 + r$	n	K_n	P
T	P_n	$\frac{2\cos\frac{\pi}{n+1}}{\left\lfloor\frac{n}{2}\right\rfloor}$	λ_1/r	$n-1$	K_n	T
R	S_n	$\sqrt{n-1}$	$\lambda_1 \cdot r$		$Bag_{p,q}$[c]	O
T	C_n	$2-n$	$\lambda_1 - g$	$n-4$	K_n	T
P	$K_{n,3}$		$\lambda_1 + g$	$n+2$	C_n	P
T	C_n	$\frac{2}{n}$	λ_1/g	$\frac{n-1}{3}$	K_n	T
P	$Ki_{n,3}$		$\lambda_1 \cdot g$	$3(n-1)$	K_n	R
T	P_n	$2\cos\left(\frac{\pi}{n+1}\right)-\frac{(3n+1)(n-1)}{4n}$ $2\cos\left(\frac{\pi}{n+1}\right)-\frac{3n-2}{4}$	$\lambda_1 - ecc$	$n-2$	K_n	T
O	S_n	$\sqrt{n-1}+2-\frac{1}{n}$	$\lambda_1 + ecc$		$K_n - E$[d]	O
T	P_n	$\frac{8n\cos\left(\frac{\pi}{n+1}\right)}{(3n+1)(n-1)}$ $\frac{8\cos\left(\frac{\pi}{n+1}\right)}{3n-2}$	λ_1/ecc	$n-1$	K_n	T
O	S_n	$\sqrt{n-1}\cdot\left(2-\frac{1}{n}\right)$	$\lambda_1 \cdot ecc$		$PK_{n,m}$[e]	O
T	P_n	$2\cos\frac{\pi}{n+1}-\frac{n+1}{4}$ $2\cos\frac{\pi}{n+1}-\frac{n^2}{4n-4}$	$\lambda_1 - \pi$	$n-2$	K_n	T
N			$\lambda_1 + \pi$	n	K_n	P
T	P_n	$\frac{8\cos\frac{\pi}{n+1}}{n+1}$ $\frac{8(n-1)\cos\frac{\pi}{n+1}}{n^2}$	λ_1/π	$n-1$	K_n	T
O	S_n	$\sqrt{n-1}$	$\lambda_1 \cdot \pi$	$n-1$	K_n	O
T	P_n	$2\cos\left(\frac{\pi}{n+1}\right)-\frac{n}{2}$	$\lambda_1 - \rho$	$n-2$	K_n	T
N			$\lambda_1 + \rho$	n	K_n	P
T	P_n	$\frac{4\cos\frac{\pi}{n+1}}{n}$	λ_1/ρ	$n-1$	K_n	T

(Continued on next page)

Table 4 *(Continued)*

N			$\lambda_1 \cdot \rho$		$PK_{n,m}$	O
P	P_n C_n	$2\cos\frac{\pi}{n+1} - \frac{n-3+2\sqrt{2}}{2}$ $(n \leqslant 9)$ $\frac{4-n}{2}$ $(n > 9)$	$\lambda_1 - Ra$	$\frac{n-2}{2}$	K_n	O
O	S_n	$2\sqrt{n-1}$	$\lambda_1 + Ra$	$\frac{3n-2}{2}$	K_n	T
P	P_n C_n	$\frac{4\cos\frac{\pi}{n+1}}{n-3+2\sqrt{2}}$ $(n \leqslant 26)$ $\frac{4}{n}$ $(n \geqslant 27)$	λ_1 / Ra	$\frac{2n-2}{n}$	K_n	O
O	S_n	$n-1$	$\lambda_1 \cdot Ra$	$\frac{n(n-1)}{2}$	K_n	T
P	K_n	-1	$\lambda_1 - a$	$n-3+t$[a]	$Ki_{n,n-1}$	O
T	P_n	$2 - 2\cos\frac{\pi}{n} + 2\cos\frac{\pi}{n+1}$	$\lambda_1 + a$	$2n-1$	K_n	T
P	K_n	$\frac{n-1}{n}$	λ_1 / a		$Ki_{n,\lfloor \frac{n}{2} \rfloor}$	O
T	P_n	$4\left(1-\cos\frac{\pi}{n}\right)\left(\cos\frac{\pi}{n+1}\right)$	$\lambda_1 \cdot a$	$n(n-1)$	K_n	T
P	K_n, C_n	0	$\lambda_1 - \nu$	$n-3+t$[a]	$Ki_{n,n-1}$	O
T	P_n	$1+2\cos\left(\frac{\pi}{n+1}\right)$	$\lambda_1 + \nu$	$2n-2$	K_n	T
P	K_n, C_n	1	λ_1 / ν	$n-2+t$[a]	$Ki_{n,n-1}$	O
T	P_n	$2\cos\left(\frac{\pi}{n+1}\right)$	$\lambda_1 \cdot \nu$	$(n-1)^2$	K_n	T
P	K_n, C_n	0	$\lambda_1 - \kappa$	$n-3+t$[a]	$Ki_{n,n-1}$	O
T	P_n	$1+2\cos\left(\frac{\pi}{n+1}\right)$	$\lambda_1 + \kappa$	$2n-2$	K_n	T
P	K_n, C_n	1	λ_1 / κ	$n-2+t$[a]	$Ki_{n,n-1}$	O
T	P_n	$2\cos\left(\frac{\pi}{n+1}\right)$	$\lambda_1 \cdot \kappa$	$(n-1)^2$	K_n	T
O	S_n	$\sqrt{n-1} - n + 1$	$\lambda_1 - \alpha$	$n-2$	K_n	T
N			$\lambda_1 + \alpha$	$\frac{n+s-1}{2} + \frac{\sqrt{(n-s-1)^2+4s(n-s)}}{2}$	$SK_{n,s}$[f]	P
N			λ_1 / α	$n-1$	K_n	T
N			$\lambda_1 \cdot \alpha$			N
P	T^*[g]	$\cos\frac{2\pi}{n+1} + \sqrt{1+\cos^2\frac{2\pi}{n+1}} - \frac{n}{2}$	$\lambda_1 - \beta$	$n-2$	K_n	T
N			$\lambda_1 + \beta$	n	K_n	P
O	T^*[g]	$\frac{2\cos\frac{2\pi}{n+1} + 2\sqrt{1+\cos^2\frac{2\pi}{n+1}}}{n}$	λ_1 / β	$n-1$	K_n	T
R	S_n	$\sqrt{n-1}$	$\lambda_1 \cdot \beta$			
P	K_n	-1	$\lambda_1 - \omega$		$\lfloor \sqrt{n} \rfloor$-partite	O
T	P_n	$2+2\cos\frac{\pi}{n+1}$	$\lambda_1 + \omega$	$2n-1$	K_n	T
O	$Ki_{n,3}$		λ_1 / ω	$\frac{1}{2}\sqrt{\lfloor \frac{n}{2} \rfloor \cdot \lceil \frac{n}{2} \rceil}$	$K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$	O
T	P_n	$4\cos\frac{\pi}{n+1}$	$\lambda_1 \cdot \omega$	$n(n-1)$	K_n	T
K	K_n	-1	$\lambda_1 - \chi$		$\lfloor \sqrt{n} \rfloor$-partite	O
T	P_n	$2+2\cos\frac{\pi}{n+1}$	$\lambda_1 + \chi$	$2n-1$	K_n	T
O	$Ki_{n,3}$		λ_1 / χ	$\frac{1}{2}\sqrt{\lfloor \frac{n}{2} \rfloor \cdot \lceil \frac{n}{2} \rceil}$	$K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$	P
T	P_n	$4\cos\frac{\pi}{n+1}$	$\lambda_1 \cdot \chi$	$n(n-1)$	K_n	T
T	P_n	$2\cos\left(\frac{\pi}{n+1}\right) - \lfloor \frac{n}{2} \rfloor$	$\lambda_1 - \mu$	$n-1-\lfloor \frac{n}{2} \rfloor$	K_n	O
O	S_n	$\sqrt{n-1}+1$	$\lambda_1 + \mu$	$n-1+\lfloor \frac{n}{2} \rfloor$	K_n	T
T	P_n	$\frac{2\cos\left(\frac{\pi}{n+1}\right)}{\lfloor \frac{n}{2} \rfloor}$	λ_1 / μ	$\sqrt{n-1}$	S_n	O
O	S_n	$\sqrt{n-1}$	$\lambda_1 \cdot \mu$	$(n-1)\lfloor \frac{n}{2} \rfloor$	K_n	T

[a] The parameter t satisfies $0 < t < 1$ and $t^3 + (2n-3)t^2 + (n^2-3n+1)t - 1 = 0$.
[b] $p = \lfloor n/2 \rfloor + 2$, $q_1 = \lceil n/4 \rceil$ and $q_2 = \lfloor (n+1)/4 \rfloor$.
[c] $p = \lfloor n/2 \rfloor + 2$ and $q = \lceil n/2 \rceil$.
[d] E is a set of $\left\lfloor \frac{n+2}{4} \right\rfloor$ disjoint edges.
[e] In this case $m = n - 2 + (k+1)k/2$ where $k = \lfloor n/2 \rfloor$.
[f] $s = \begin{cases} \left\lceil \frac{n+1+\sqrt{n^2-n+1}}{3} \right\rceil & (n \equiv 1[3]), \\ \left\lfloor \frac{n+1+\sqrt{n^2-n+1}}{3} \right\rfloor & (n \not\equiv 1[3]). \end{cases}$
[g] T^* is the tree obtained from a path on $n/2$ (n must be even) vertices by attaching a pending edge to each vertex.

Table 5
AGX Form 1 conjectures about the algebraic connectivity a.

S	G for l_n	l_n	$a \oplus I$	u_n	G for u_n	S
P	S_n	$2-n$	$a-\Delta$	1	K_n	P
T	P_n	$4-2\cos\frac{\pi}{n}$	$a+\Delta$	$2n-1$	K_n	T
O	Comet		a/Δ	$\frac{n}{n-1}$	K_n	P
T	P_n	$4-4\cos\frac{\pi}{n}$	$a\cdot\Delta$	$n(n-1)$	K_n	T
O	$Ki_{n,n-1}$	$4-n-\frac{4}{n}$	$a-\bar{d}$	1	K_n	P
T	P_n	$4-\frac{2}{n}-2\cos\frac{\pi}{n}$	$a+\bar{d}$	$2n-1$	K_n	T
O	Kite		$a/\bar{d}$	$\frac{n}{n-1}$	K_n	P
T	P_n	$\left(4-\frac{4}{n}\right)\left(1-\cos\frac{\pi}{n}\right)$	$a\cdot\bar{d}$	$n(n-1)$	K_n	T
O	$K\left(\frac{n}{2},\frac{n}{2}\right)$[a]		$a-\delta$	1	K_n	K
T	P_n	$3-2\cos\frac{\pi}{n}$	$a+\delta$	$2n-1$	K_n	T
O	TPT[b]		a/δ	$\frac{n}{n-1}$	K_n	K
T	P_n	$2-2\cos\frac{\pi}{n}$	$a\cdot\delta$	$n(n-1)$	K_n	T
T	P_n	$2-2\cos\frac{\pi}{n}-\frac{n+1}{3}$	$a-\bar{l}$	$n-1$	K_n	T
O	$Ki_{n,n-2}$		$a+\bar{l}$	$n+1$	K_n	P
T	P_n	$6\frac{1-\cos\frac{\pi}{n}}{n+1}$	$a/\bar{l}$	n	K_n	T
O	TPT[b]		$a\cdot\bar{l}$	n	K_n	P
T	P_n	$3-n-2\cos\frac{\pi}{n}$	$a-D$	$n-1$	K_n	T
O	S_n	3	$a+D$	$n+1$	K_n	P
T	P_n	$\frac{2}{n-1}\left(1-\cos\frac{\pi}{n}\right)$	a/D	n	K_n	T
O	$DC_{n,\Delta,\Delta}$[c]		$a\cdot D$	$2n-4$	$\bar{E}$[d]	P
T	P_n	$2\left(1-\cos\left(\frac{\pi}{n}\right)\right)-\left\lfloor\frac{n}{2}\right\rfloor$	$a-r$	$n-1$	K_n	T
P	S_n	2	$a+r$	$n+1$	K_n	P
T	P_n	$\frac{2(1-\cos\frac{\pi}{n})}{\lfloor\frac{n}{2}\rfloor}$	a/r	n	K_n	T
N			$a\cdot r$	$4\left\lfloor\frac{n}{2}\right\rfloor-4$	$\bar{S}$[e]	P
P	C_n	$2\left(1-\cos\frac{2\pi}{n}\right)-n$	$a-g$	$n-3$	K_n	T
O	$Ki_{n,3}$		$a+g$	$n+3$	K_n	P
O	$Lol_{n,\lfloor\frac{n}{2}\rfloor}$		a/g	$\frac{n}{3}$	K_n	T
O	$Ki_{n,3}$		$a\cdot g$	$3n$	K_n	P
T	P_n	$2-2\cos\frac{\pi}{n}-\frac{3n+1}{4}\frac{n-1}{n}$ (n odd) $2-2\cos\frac{\pi}{n}-\frac{3n-2}{4}$ (n even)	$a-ecc$	$n-1$	K_n	T
P	S_n	$3-\frac{1}{n}$	$a+ecc$	$n+1$	K_n	P
T	P_n	$\frac{(3n+1)(n-1)}{8n(1-\cos\frac{\pi}{n})}$ (n odd) $\frac{3n-2}{8(1-\cos\frac{\pi}{n})}$ (n even)	a/ecc	n	K_n	P
O	Double comet		$a\cdot ecc$	$2n-\frac{5n-2}{n}$ (n odd) $2n-4$ (n even)	$\bar{M}$[f]	P
T	P_n	$2-2\cos\frac{\pi}{n}-\frac{3n+1}{4}\frac{n-1}{n}$ (n odd) $2-2\cos\frac{\pi}{n}-\frac{3n-2}{4}$ (n even)	$a-\pi$	$n-1$	K_n	T
N			$a+\pi$	$n+1$	K_n	P
T	P_n	$\frac{8n(1-\cos\frac{\pi}{n})}{(3n+1)(n-1)}$ (n odd) $\frac{8(1-\cos\frac{\pi}{n})}{3n-2}$ (n even)	a/π	n	K_n	T
O	P_n	$\frac{3n+1}{2}\frac{n-1}{n}\left(1-\cos\frac{\pi}{n}\right)$ (n odd) $\frac{3n-2}{2}\left(1-\cos\frac{\pi}{n}\right)$ (n even)	$a\cdot\pi$	n	K_n	P
T	P_n	$2-2\cos\frac{\pi}{n}-\frac{n}{2}$	$a-\rho$	$n-1$	K_n	T
O	$K(\frac{n}{2},\frac{n}{2})$[a]		$a+\rho$	$n+1$	K_n	P
T	P_n	$\frac{4(1-\cos\frac{\pi}{n})}{n}$	a/ρ	n	K_n	T
O	$KPK_{n,p,q}$[g]		$a\cdot\rho$	n	K_n	P
N			$a-Ra$	$\frac{n}{2}$	K_n	O

(Continued on next page)

Table 5 (*Continued*)

N	Comet		$a+Ra$	$\frac{3n}{2}$	K_n	T
O	P_n	$\frac{4(1-\cos\frac{\pi}{n})}{n-3+2\sqrt{2}}$	a/Ra	2	K_n	O
O	Double comet		$a \cdot Ra$	$\frac{n^2}{2}$	K_n	T
O	$Ki_{n,n-1}$	$3-n-t$[j]	$a-\lambda_1$	1	K_n	P
T	P_n	$2-2\cos\frac{\pi}{n}+2\cos\frac{\pi}{n+1}$	$a+\lambda_1$	$2n-1$	K_n	T
O	$Ki_{n,\lfloor\frac{n}{2}\rfloor}$		a/λ_1	$\frac{n}{n-1}$	K_n	P
T	P_n	$\left(2-2\cos\frac{\pi}{n}\right)\left(2\cos\frac{\pi}{n+1}\right)$	$a \cdot \lambda_1$	$n(n-1)$	K_n	T
N			$a-\nu$	1	K_n	K
T	P_n	$3-2\cos\frac{\pi}{n}$	$a+\nu$	$2n-1$	K_n	T
O	P_n	$2-2\cos\frac{\pi}{n}$	a/ν	$\frac{n}{n-1}$	K_n	K
T	P_n	$2-2\cos\frac{\pi}{n}$	$a \cdot \nu$	$n(n-1)$	K_n	T
N			$a-\kappa$	1	K_n	K
T	P_n	$3-2\cos\frac{\pi}{n}$	$a+\kappa$	$2n-1$	K_n	T
O	P_n	$2-2\cos\frac{\pi}{n}$	a/κ	$\frac{n}{n-1}$	K_n	K
T	P_n	$2-2\cos\frac{\pi}{n}$	$a \cdot \kappa$	$n(n-1)$	K_n	T
P	S_n	$2-n$	$a-\alpha$	$n-1$	K_n	T
O	$KeK_{p,n-p}$[h]		$a+\alpha$	$n+1$	K_n	P
O	Double comet		a/α	n	K_n	T
O	$KPK_{n,p,q}$		$a \cdot \alpha$	$\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil$	$K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$	P
N			$a-\beta$	$n-1$	K_n	T
P	S_n	2	$a+\beta$	$n+1$	K_n	P
N			a/β	n	K_n	T
P	S_n	1	$a \cdot \beta$	$4\lfloor\frac{n}{2}\rfloor-4$	$\overline{F}$[i]	O
P	$2-n$	$Ki_{n,n-1}$	$a-\omega$	$\left\lfloor n-\frac{n}{\lfloor\sqrt{n}\rfloor}\right\rfloor-\lfloor\sqrt{n}\rfloor$	$\sqrt{n}$-partite	O
T	P_n	$4-2\cos\frac{\pi}{n}$	$a+\omega$	$2n$	K_n	T
O	$Ki_{\lfloor\frac{n}{2}\rfloor}$		a/ω	$\frac{1}{2}\lfloor\frac{n}{2}\rfloor$	$K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$	O
T	P_n	$4-4\cos\frac{\pi}{n}$	$a \cdot \omega$	n^2	K_n	T
P	$2-n$	$Ki_{n,n-1}$	$a-\chi$	$\left\lfloor n-\frac{n}{\lfloor\sqrt{n}\rfloor}\right\rfloor-\lfloor\sqrt{n}\rfloor$	$\sqrt{n}$-partite	O
T	P_n	$4-2\cos\frac{\pi}{n}$	$a+\chi$	$2n$	K_n	T
O	$Ki_{\lfloor\frac{n}{2}\rfloor}$		a/χ	$\frac{1}{2}\lfloor\frac{n}{2}\rfloor$	$K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$	P
T	P_n	$4-2\cos\frac{\pi}{n}$	$a+\chi$	$2n$	K_n	T
T	P_n	$2-2\cos\frac{\pi}{n}-\lceil\frac{n}{2}\rceil$	$a-\mu$	$\lceil\frac{n}{2}\rceil$	K_n	T
P	S_n	2	$a+\mu$	$n+\lfloor\frac{n}{2}\rfloor$	K_n	T
T	P_n	$\frac{2-2\cos\frac{\pi}{n}}{\lceil\frac{n}{2}\rceil}$	a/μ	$\frac{n}{\lfloor\frac{n}{2}\rfloor}$	K_n	O
P	S_n	1	$a \cdot \mu$	$n \cdot \lfloor\frac{n}{2}\rfloor$	K_n	T

[a] $K(\frac{n}{2},\frac{n}{2})$ is the graph from two cliques on $\lceil n/2\rceil$ vertices each by a coalescence of two vertices, one of each clique, if n is odd, or by adding an edge between the two cliques if n is even.

[b] TPT is the graph composed of two triangles linked by a path.

[c] DC_{n,Δ_1,Δ_2} is a double comet on n vertices with degrees Δ_1 and Δ_2, *i.e.*, the tree obtained from two stars S_{Δ_1} and S_{Δ_2} by linking between their central vertices using a path. Here $\Delta_1=\Delta_2=\Delta=\lceil\frac{n+1}{3}\rceil$.

[d] E is any nonempty set of disjoint edges.

[e] S is a perfect matching if n is even, and E is a set of connected components in $\overline{G}$ on at least 2 and at most 3 vertices each.

[f] M is a matching on $\lfloor n/2\rfloor$ edges.

[g] $KPK_{n,p,q}$ is the graph obtained from two cliques on K_p and K_q by adding a path between two vertices, one from each clique. For the lower bound on $a \cdot \rho$ we have $p=q=\lceil\frac{n}{3}\rceil$.

[h] $KeK_{p,n-p}$ is the graph obtained from two cliques on K_p and K_{n-p} by adding an edge between two vertices, one from each clique. In our case $p=\left\lfloor\frac{n}{2}\right\rfloor$.

[i] F is a set of $\lceil n/2\rceil$ edges covering all the vertices.

[j] The parameter t satisfies $0<t<1$ and $t^3+(2n-3)t^2+(n^2-3n+1)t-1=0$.

Table 6
Graffiti conjectures related to graph spectra.

#	Conjecture	S	#	Conjecture	S
	For any graph G			For any graph G	
19	$-\lambda_n \leqslant Ra$	P	20	$p^+ \leqslant \sum_{\lambda_i>0} \lambda_i$	O
21	$p^- \leqslant \sum_{\lambda_i>0} \lambda_i$	O	22	$-\max(\Lambda^-) \leqslant \alpha$	R
24	$Mn(Tp) \leqslant p^-$	P	25	$Mn(Tp) \leqslant p^-(\mathcal{D})$	P
28	$Ra \leqslant \sum_{\lambda_i>0} \lambda_i$	R	29	$Ra \leqslant p^-(\mathcal{D})$	R
30	$p^+(\mathcal{D}) \leqslant \sum_{v\in V} Tp(v)$	R	31	$-\max(\Lambda^-(\mathcal{D})) \leqslant \alpha$	R
32	$-\max(\Lambda^-(\mathcal{D})) \leqslant \mu$	O	33	$-\max(\Lambda^-(\mathcal{D})) \leqslant \chi$	R
35	$D \leqslant -\max(\Lambda^-(\mathcal{D}))$	P	36	$D \leqslant p^-(\mathcal{D})$	P
37	$r \leqslant \sum_{\lambda_i>0} \lambda_i$	P	38	$var(\mathcal{D}) \leqslant -\lambda_n$	P
39	$dev(\mathcal{D}) \leqslant p_+$	O	40	$dev(\mathcal{D}) \leqslant p_-$	O
128	$a \leqslant n/\bar{l}$	P	129	$dev(\Lambda(L)) \leqslant Ra$	O
137	$\lambda_2 \leqslant Hc$	R	138	$\lambda_2 \leqslant m/\omega$	P
139	$-\lambda_{n-1} \leqslant Hc$	R	140	$dev(\Lambda) \leqslant Hc$	R
141	$p_+ \leqslant \mu$	R	142	$\min(\Lambda^+) \leqslant n/\bar{l}$	O
143	$var(\Lambda^+) \leqslant m/\bar{l}$	O	144	$var(\Lambda^+) \leqslant m-\mu$	O
145	$\min((\Lambda^+)') \leqslant n/\bar{l}$	R	146	$\sum_{\lambda_i>0} \lambda_i \leqslant m$	P
150	$\min(\Lambda'(Gr)) \leqslant n/\alpha$	O	151	$p_+(Gr) \leqslant \mu$	O
154	$dev(\Lambda) \leqslant n/\bar{l}$	O	160	$-\lambda_n \leqslant \sqrt{m}$	P
162	$\chi/\omega \leqslant p_+$	O	165	$Md(\Lambda(L)) \leqslant m/\bar{l}$	R
166	$\sqrt{m} \leqslant p_-(\mathcal{D}) + p_0(\mathcal{D})$	R	167	$\sum_{i=1}^n 1/\mu_i \leqslant Mn(t)$	P
168	$\min(\Lambda'(L)) \leqslant n/\alpha$	O	172	$\min(\Lambda') \leqslant n/\alpha$	O
173	$n/\bar{l} \leqslant \lVert\Lambda(L)\rVert$	O	178	$-\lambda_{n-1} \leqslant \mu$	R
252	$\min(\Lambda'(L)) \leqslant \sum_{v\in V} 1/d^*(v)$	O	253	$dev(\Lambda(L)) \leqslant \Delta^*$	P
254	$\min(\Lambda'(L)) \leqslant \sum_{v\in V} 1/Od(v)$	O	256	$\lambda_1 \leqslant \Delta^*$	P
258	$p_+ \leqslant \mu + \bar{\mu}$	P	262	$-\lambda_1 \leqslant \max(Ev)$	O
263	$Rg(maxine) \leqslant 1 + Rg(\Lambda^+)$	O	264	$2 + Rg(\Lambda^+) \leqslant \chi + \bar{\chi}$	R
265	$2 - \lambda_n \leqslant \chi + \bar{\chi}$	R	543	$n - \alpha \leqslant \sum_{\lambda_i>0} \lambda_i$	O
568	$p_+ - p_- \leqslant m/\alpha$	O	694	$\exists Vec(\lambda_n) : \max(Vec) \leqslant \alpha$	O
696	$Mn(\overline{\Lambda^+}) \leqslant \bar{\chi}$	O	697	$Rg(Vec(\lambda_1)) \leqslant n - m_1$	O
698	$\lVert\Lambda^-\rVert \leqslant Ra$	O	706	$\mu \leqslant \sum_{\lambda_i>0} \lambda_i$	P
707	$r \leqslant \lvert\{Vec_i(\lambda_n) : Vec_i(\lambda_n) > 0\}\rvert$	O	708	$\bar{l} \leqslant Vec(\lambda_n) \cdot Vec(\lambda_n)$	O
709	$\max(Vec(\lambda_1) \leqslant Rs$	O	711	$Rg(Def) \leqslant Rg(\Lambda)$	R
712	$\min(Tp) \leqslant p_- + p_0$	O	713	$-Mn(\overline{\Lambda^+}) \leqslant Ra$	P
714	$-Mn(\overline{\Lambda^+}) \leqslant \sum_{v\in V} 1/Tp(v)$	O	715	$Sp(\overline{\Lambda^+}) \leqslant Mn(\{d_i : d_i \geqslant \bar{d}\})$	R
722	$p_- + p_0 + \sum_{\lambda_i<0} 1/\lambda_i \leqslant \alpha$	R	723	$p_0 + p_+ - \sum_{v\in V} Tp(v) \leqslant \alpha$	R
724	$p_0 + p_+ - \lambda_1 + \min(\Lambda^+) \leqslant \alpha$	R	725	$p_0 + p_+ - \sum_{v\in V} 1/Mx(v) \leqslant \alpha$	R
778	$jet^f \leqslant p_+$	P	792	$\alpha \leqslant 1 + \overline{\lambda_1}$	P
	For G regular			For G regular	
43	$-\lambda_n \leqslant \mu$	P	44	$\lambda_2 \leqslant \alpha$	R
45	$\lambda_2 \leqslant \mu$	P	46	$\min\{\lambda_i : \lambda_i > 0\} \leqslant \lvert\text{Center}\rvert$	R
47	$\min\{\lambda_i : \lambda_i > 0\} \leqslant \lvert\text{Boundary}\rvert$	R	48	$\sum_{\lambda_i>0} \lambda_i \leqslant \lambda_1(\mathcal{D})$	P
49	$-\max\{\lambda_i : \lambda_i < 0\} \leqslant \min(req(\mathcal{D}))$	O	50	$p_0 \leqslant \min Md(\mathcal{D})$	P
51	$p_0 \leqslant \lvert\text{Center}\rvert$	P	52	$p_0 \leqslant \lvert\text{Boundary}\rvert$	P
55	$\lambda_2 \leqslant \min Md(\mathcal{D})$	R	56	$\lambda_2 \leqslant \lvert\text{Center}\rvert$	R
58	$-\max\{\lambda_i : \lambda_i < 0\} \leqslant \lvert\text{Center}\rvert$	R	59	$D \leqslant \sum_{\lambda_i>0} \lambda_i$	R
233	$\max(\Lambda'(L)) \leqslant n/\bar{l}$	O	422	$n - \sum_{\lambda_i>0} \lambda_i \leqslant \alpha$	O
	For G triangle-free			For G triangle-free	
116	$\lambda_1 \leqslant Ra$	P	215	$m/\alpha \leqslant Sp(\Lambda)$	R
218	$\lambda_1 \leqslant \sqrt{m}$	P	219	$\lambda_2(Gr) \leqslant n(n-1)/2 - m$	O
312	$m/\alpha \leqslant p_+ + p_0$	O	313	$m/\alpha \leqslant p_-(\mathcal{D})$	O

(*Continued on next page*)

Table 6 (*Continued*)

#	Conjecture	S	#	Conjecture	S
316	$\chi \leqslant Rg(\Lambda(L))$	O	319	$\max(\Lambda'(L)) \leqslant \sum_{v\in V} 1/Rw(v)$	O
321	$\lambda_1 \leqslant Mn(Ev)$	R	322	$\sum_{v\in V} 1/Ev(v) \leqslant Rg(\Lambda(\mathcal{D}))$	O
323	$Sp(\Lambda^+) \leqslant \bar{\mu}$	O			
	If $\sum_{v\in V} Od(v) \leqslant \sum_{v\in V} Ev(v)$			If $\sum_{v\in V} Od(v) \leqslant \sum_{v\in V} Ev(v)$	
186	$m/\alpha \leqslant E$	R	187	$Md(\Lambda(L)) \leqslant n - \alpha$	R
188	$Md(\Lambda(L)) \leqslant n - \mu$	R	189	$Md(\Lambda(L)) \leqslant p_- + p_0$	R
190	$dev(\Lambda(L)) \leqslant Mn(Ev)$	P	194	$\lambda_1 \leqslant m/\bar{l}$	R
195	$\lambda_1 \leqslant \max(Ev)$	O	196	$\lambda_2 \leqslant Mn(Ev)$	P
197	$-\lambda_{n-1} \leqslant Rg(\Lambda(Gr))$	O	198	$\min(\Lambda) \leqslant n/Mn(Gr)$	O
199	$-\lambda_n \leqslant Mn(Ev)$	P	200	$\min\{\lambda_i : \lambda_i > 0\} \leqslant Ra$	P
201	$\min(\Lambda^+) \leqslant m/\omega$	R			
	If $\sum_{v\in V} Ev(v) \leqslant \sum_{v\in V} Od(v)$			If $\sum_{v\in V} Ev(v) \leqslant \sum_{v\in V} Od(v)$	
206	$\lambda_2 \leqslant \mu$	R	207	$-\lambda_n \leqslant \mu$	R
208	$-\lambda_n \leqslant Hc$	P	209	$\sum_{\lambda_i>0} \lambda_i \leqslant Mn_{v\in V} t(v)$	R
210	$\bar{l} \leqslant p_-(Gr)$	O	211	$n/\bar{l} \leqslant E$	P
662	$dev(\Lambda) \leqslant n - \alpha$	O			
	For G with $g \geqslant 5$			For G with $g \geqslant 5$	
223	$a \leqslant n/\alpha$	O	281	$\max\{\mu, \bar{\mu}\} \leqslant p_-(\mathcal{D})$	R
283	$\alpha \leqslant p_-(\mathcal{D}) + p_0(\mathcal{D})$	O	284	$\delta^* \leqslant -\lambda_n(\mathcal{D})$	O
286	$\mu_2 \leqslant \mu + \bar{\mu}$	O	287	$a \leqslant \sum_{v\in V} 1/d^*(v)$	O
289	$\lambda_2 \leqslant \overline{d^*}$	R	290	$-\lambda_{n-1} \leqslant m/Mn(Gr)$	O
291	$Sp(\Lambda^+) \leqslant m/Mn(Gr)$	O	292	$\min(\Lambda^+) \leqslant n/Mn(Gr)$	O
293	$\min((\Lambda^+)') \leqslant m/\alpha$	R	294	$p_+(\mathcal{D}) \leqslant n/Mn(Gr)$	O
	For G K_4-free			For G K_4-free	
241	$m/\alpha \leqslant Sp(\Lambda)$	R	243	$m/\alpha \leqslant \mu_1$	R
244	$dev(\Lambda(L)) \leqslant n/2$	R			
	If G is a tree			If G is a tree	
297	$a \leqslant n/\alpha$	P	301	$Sp(\Lambda^+) \leqslant Hc$	R
302	$Sp(\Lambda^+) \leqslant \overline{d^*}$	R			
	For G with $Rk(\mathcal{D}) \leqslant Rk(A)$			For G with $Rk(\mathcal{D}) \leqslant Rk(A)$	
305	$\sum_{v\in V} 1/d^*(v) \leqslant p_+ + p_0$	R	306	$\sum_{v\in V} 1/d^*(v) \leqslant p_- + p_0$	R
307	$\bar{l} \leqslant n/\lambda_1$	R	578	$r \leqslant Rg(\Lambda^+)$	P
584	$\mu_1 \leqslant 2 + \alpha$	P			
	If G is a plant			If G is a plant	
346	$\bar{l} \leqslant Rg(\Lambda(\mathcal{D}))$	O	348	$\min \lambda_{i+1} - \lambda_i \leqslant Mn(Gr)$	O
	If G is a heliotropic plant			If G is a heliotropic plant	
351	$r \leqslant p_+$	O	720	$Ra \leqslant p_- + p_0$	P
	If G is a geotropic plant				
356	$r \leqslant p_-$	O			
	For G with $\alpha \leqslant 2$			For G with $\alpha \leqslant 2$	
399	$Rg(\Lambda^+) \leqslant \mu$	O	400	$Rg(\Lambda^+) \leqslant \Delta^*$	O
401	$\min((\Lambda^+)') \leqslant Mn(Gr)$	R	402	$n/\bar{l} \leqslant \mu_1$	O
403	$n/\bar{l} \leqslant Sp(\Lambda)$	R	404	$\lambda_2(\mathcal{D}) \leqslant tr^{\mathrm{b}}$	O
404'	$\lambda_2(\mathcal{D}) \leqslant m/Mn(Gr)$	O	405	$-\lambda_n(\mathcal{D}) \leqslant \mu + \bar{\mu}$	R
	If G is the $RP[2, \cdots k]$			If G is the $RP[2, \cdots k]$	
434	$\mu_2 = k - 1$	P	446	$p_0 + p_+ = pr(k)^{\mathrm{c}}$	P
454	$pr(k) \leqslant Rg(\Lambda)$	O			
	If G is $RP[S]$			If G is $RP[S]$	
470	$p_0 + p_+ = pr(k)$	O	800	$\alpha \leqslant 1 + \overline{p_-} + \overline{p_0}$	P
802	$\alpha \leqslant \text{Turanbound} + \lambda_1 - \lambda_2$	O	804	$\alpha \geqslant uq^{\mathrm{d}} + \lvert\{\lambda_i : \lambda_i \geqslant 1\}\rvert$	O
805	$\lambda_1 \leqslant 1 + \sum_{v\in V} Tp(v)$	O	806	$\lambda_1 \leqslant Rg(d_1, \cdots d_n)$	O
807	$\lambda_2 \leqslant \lambda_1/2$	O	808	$\lambda_1 \geqslant \overline{d^*}$	O
809	$p_+ \leqslant r - 1$	O	810	$\lambda_2 \geqslant$	O

Table 6 (*Continued*)

811	$\lambda_2 \geqslant freq(\Delta) \cdot jet$	O	812	$\lambda_1 - \lambda_2 \leqslant dev(d_1, \cdots d_n) + p_-/p_+$	O
813	$\lambda_1 - \lambda_2 \leqslant dev(d_1, \cdots d_n) + Mn(Tp)$	O			
	If G is a Paley graph			If G is a Paley graph	
509	$Mn(Rw) \leqslant freq(\mu_1)$	O	516	$dev(S) \leqslant freq(Md(\Lambda(L)))$	O
523	$Md(\Lambda(L)) \leqslant nb$[a]	O			
	For a connected Caylay graph				
538	$\max(Rw) \leqslant p_-$	O			
	For G with $\bar{\chi} = n - \mu$			For G with $\bar{\chi} = n - \mu$	
636	$m/\alpha \leqslant \mu_1$	P	637	$m/\alpha \leqslant \sum_{\lambda_>0} \lambda_i$	R
649	$\exists G : \bar{\chi}/\alpha \geqslant Rg(\Lambda^+)$	R	650	$\lambda_1 \leqslant \chi + \bar{\chi}$	O
	If G is a cubic graph			If G is a cubic graph	
771	$\alpha \leqslant p_0 + p_+ - D$	R	774	$\alpha \geqslant \lvert\{\lambda_i : \lambda_i > 1\}\rvert$	P
776	$\alpha \geqslant -1 + \frac{1}{2} \sum_{\lambda_i>0} \lambda_i$	R	850	If $g = 5$ then $p_- \leqslant 1 + \min(Od)$	O
	If G is a fullerene			If G is a fullerene	
841	$p_+ \geqslant p_-$	R	844	$\alpha \geqslant \lvert\{\lambda_i : \lambda_i \geqslant -1\}\rvert$	O
845	$\sum_{\lambda_i>0} \lambda_i \leqslant 1 + \alpha_2$	O	846	$\sum_{\lambda_i>0} \lambda_i \leqslant 1 + p_+ - \lambda_n(\overline{G})$	O
847	mr[e] $+ 2.7 \leqslant \sum_{\lambda_i>0} \lambda_i$	O	848	$p_- \leqslant Mn(Ev)$	O
849	$p_- \leqslant Ev(v)$	O	852	$p_- \geqslant \max HE$[g]	O
855	$p_+ \geqslant 2(\max HE - \min HE)$	O	856	$\sum_{\lambda_i>0} \lambda_i \geqslant 1 + \lvert\{\lambda_i : \lambda_i \geqslant -1\}\rvert$	O
	If G is an IP isomer			If G is an IP isomer	
860	$\sum_{\lambda_i>0} \lambda_i \leqslant \alpha_2 - 1$	O	861	$\sum_{\lambda_i>0} \lambda_i \geqslant 3n/4 + 1.6$	O

[a] nb the number of square-free integers not greater than n.
[b] tr number of triangles in a graph.
[c] $pr(k)$ is the number of primes less or equal k.
[d] uq is the upper quotient of the degree sequence of a graph.
[e] mr is the minimum possible response of the second player for all possible moves of the first player in a market game [50].
[f] jet is the jet number of a graph , *i.e.*, the number of vertices of a smallest set such that the complement of its span is a maximum independent set.
[g] HE is the number of horizontal edges with respect to a given representation of a fullerene.

derivative Vec' of a nonincreasing vector Vec is defined by $Vec'(i) = Vec(i) - Vec(i+1)$. The length $||Vec||$ of a vector Vec is its euclidian norm, *i.e.*, $||Vec|| = \sqrt{Vec_1^2 + Vec_2^2 + \cdots Vec_n^2}$. We denote by Vec^+ and Vec^- the vectors composed of positive and negative components of Vec respectively, and by $\overline{Vec^+}$ and $\overline{Vec^-}$ the vectors composed of nonpositive and nonnegative components of Vec respectively. For a given matrix M, we use $\Lambda(M)$ to denote the vector of eigenvalues of M, and when M is not specified Λ denotes the eigenvalue vector of (the adjacency matrix of) the graph. The variance and deviation of a vector Vec are denoted by $var(Vec)$ and $dev(Vec)$ respectively. The *variance* $var(Vec)$ of a vector Vec is defined by $var(Vec) = \left(\sum_{i=1}^n (Vec_i - Mn(Vec))\right)/n$. The *standard deviation* is defined by $dev(Vec) = \sqrt{var(Vec)}$. Let $G = (V, E)$ a simple graph and $v \in V$. The *temperature* of the vertex v is defined by $Tp(v) = d(v)/(n - d(v))$ where $d(v)$ denotes the degree of v. The temperature of a graph G, denoted by $Tp = Tp_G$ is the vector of the temperatures of its vertices. The *dual degree* $d^*(v)$ of a vertex v is the average degree of its neighbors. The minimum, average and maximum dual degree are denoted by δ^*, $\overline{d^*}$ and Δ^* respectively. The *harmonic* of a graph G is $Hc(G) = \sum_{uv \in E} 1/(d(u) + d(v))$. The *gravity matrix* $Gr = Gr(G)$ of a graph G is the square matrix indexed by the vertices of G and $Gr_{uv} = 0$ if $u = v$ or when there is not path joining u and v, otherwise $Gr_{uv} = (d(u) \cdot d(v) \cdot d(u, v))$. The *deficiency vector* $def = def(G)$ of a graph G is the vector indexed by the vertices of G in which Def_v is the number of nonedges in the graph induced by the neighbors of vertex v. The *odd vector* $Od = Od(G)$ (resp. *even vector* $Ev = Ev(G)$) of the graph G is the vector indexed by the vertices of G where $Od(v)$ (resp. $Ev(e)$) is the number of vertices at odd (resp. even) distances from v. The *rainbow* $Rw = Rw(G)$ of a graph G is the vector indexed by the vertices of G where $Rw(v)$ is the number of colors used for the neighbors of v for given χ-coloration. The *residue* $Rs = Rs(G)$ of a graph G of a degree sequence $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, is the number of zeros obtained by the iterative process consisting, while $d_1 \neq 0$, in deleting the first term d_1 of the sequence, subtracting 1 from the d_1 following ones and sorting down the new sequence.

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