Discussiones Mathematicae
Graph Theory 29 (2009) 15–37

VARIABLE NEIGHBORHOOD SEARCH FOR EXTREMAL GRAPHS. 17. FURTHER CONJECTURES AND RESULTS ABOUT THE INDEX*

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Abstract

The AutoGraphiX 2 system is used to compare the index of a connected graph G with a number of other graph theoretical invariants, i.e., chromatic number, maximum, minimum and average degree, diameter, radius, average distance, independence and domination numbers. In each case, best possible lower and upper bounds, in terms of the order of G, are sought for sums, differences, ratios and products of the index and another invariant. There are 72 cases altogether:

*This work has been supported by NSERC Grant 105574–2002 and the Data Mining Chair of HEC Montréal, Canada. The third author acknowledges partial support by Grant 144015G of Serbian Ministry of Science.

in 7 cases known results were reproduced, in 32 cases immediate results were obtained and automatically proved by the system, conjectures were obtained in 27 cases, of which 12 were proved (in 3 theorems and 9 propositions), 9 remain open and 6 were refuted. No results could be derived in 7 cases.

Keywords: AutoGraphiX, automated conjecture making, index of a graph, spectral radius, graph invariant.

2000 Mathematics Subject Classification: 05C35, 05C50, 05C75.

1. Introduction

The role of the computer in graph theory is rapidly increasing, see e.g. [10, 14, 15, 16] for surveys and discussions. To the traditional tasks of invariant computation, graph drawing and graph enumeration by computer, several others have been added. The *AutoGraphiX* (AGX) system [7, 8] addresses the following: (i) find a graph satisfying given constraints, (ii) find a graph with a maximum (minimum) value for some invariant, possibly subject to constraints, (iii) strengthen, corroborate or refute a conjecture, (iv) find new conjectures, (v) find ideas of proofs. Recently a new version, AGX 2, of this system has been developed [2]. Its interactive features, i.e., online graph representation and modification, computation of invariants and language for easy formulation of problems have been much improved, as well as the Variable Neighborhood Search [22] heuristic on which it relies. Moreover, some simple results in fully automated theorem proving of graph theory conjectures have been obtained. To evaluate these new features, a systematic comparison among 20 graph invariants (i.e., quantities not depending on the numbering of the edges or vertices) for the class of all connected graphs $G = (V, E)$ has been conducted [1, 3]. Precisely, one seeks relations of the form:

$$b_1(n) \leq i_1(G) * i_2(G) \leq b_2(n),$$

where $*$ is one of $+$, $-$, $\cdot$ and $/$, $i_1(G)$ and $i_2(G)$ are graph invariants, and $b_1(n)$ and $b_2(n)$ are bounds expressed as functions of the order $n = |V|$ of G; in addition it is asked that these bounds be best possible in the strong sense that for each value of n (≥ 3 to avoid border effects) there exist at least one graph for which the bound is tight. Finally, a characterization of extremal graphs is requested.

It turns out that this class of problems exhibits the whole range of difficulties of finding conjectures in graph theory, from elementary observations to some apparently hard open conjectures. Results obtained are explicit conjectures in algebraic form and/or structural conjectures about the class of extremal graphs. Easy explicit conjectures can be solved by the automated theorem proving component of AGX 2; the other ones may be proved by hand, or remain open. Structural conjectures can be transformed into explicit ones by manipulations of formulae from a database specifying values of invariants as functions of n. In some cases, these formulae are parametric and it is necessary to proceed to some optimization to get the derived form.

The following cases occur:

(i) *Fully automated results:* explicit formulae are obtained, together with their proof and a characterization of the corresponding extremal graphs. Such results are usually easy to prove, they are called *observations*;

(ii) *Fully automated conjectures:* as in (i) but without automated proof. If a manual proof is obtained these results are referred to as *propositions* or *theorems* according to the difficulty of the proof;

(iii) *Derived conjectures:* structural conjectures from which explicit relations can be obtained manually. They are divided in *optimized* and *non-optimized* conjectures according to the fact that some parameters are optimized or not;

(iv) *Structural conjectures:* as in (iii) but without finding explicit relations because they are too hard to obtain or do not exist;

(v) *No results:* No best possible bounds or families of extremal graphs could be found.

Results are reported on in [1] and summarized in [3]. In this paper, we examine in more detail the case of one invariant, the index λ_1 of the adjacency matrix of a graph, compared to several others, i.e., the chromatic number χ, the maximum degree Δ, the minimum degree δ, the average degree $\bar{d}$, the diameter D, the radius r, the average distance $\bar{l}$ between pairs of distinct vertices, the independence number α and the domination number β (see e.g. [5] for definitions). Altogether, 72 cases are examined, details of which are given below. Several conjectures are presented as theorems and proved in Section 2. A number of further conjectures lead to propositions given in Section 3. In Section 4, we first give a list of open conjectures, and then discuss refuted ones. Section 5 contains conclusions. In an appendix, Table 1 summarizes all the results discussed in this paper.

Throughout the paper it is assumed that, whenever mentioned, G is a simple, connected graph with $n \geq 3$ vertices. We also assume a certain level of familiarity with graph theory from the reader. Otherwise, for a good introduction to graph theory, see [5]. However, we need to define (or recall the definition of) a few special graph classes that appear as extremal graphs in a number of conjectures:

A *short lollipop* SL_n is a graph obtained from a cycle on $n-1$ vertices by attaching a pendant edge to one of its vertices.

A *short kite* SK_n is a graph obtained from a clique on $n-1$ vertices by attaching a pendant edge to one of its vertices.

A *pineapple graph* $PA_{n,k}$ is a graph obtained from a clique on $n-k$ vertices by attaching k pendant edges to one of its vertices.

A *complete split graph* $S_{n,\alpha}$ is a graph obtained from an empty graph on α vertices and a clique on $n-\alpha$ vertices by adding all edges between them.

A *bag* $Bag_{p,q}$ is a graph on $p+q-2$ vertices 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*.

A *bug* Bug_{p,q_1,q_2} is a graph on $p+q_1+q_2-2$ vertices obtained from a complete graph K_p by deleting an edge uv and attaching paths P_{q_1} and P_{q_2} at u and v, respectively. A bug is called *balanced* if $|q_1-q_2| \leq 1$.

A *caterpillar* is a tree T which consists of a path P and a number of pendant vertices attached to inner vertices of the path.

2. THEOREMS

In this section, we present the three main results of this paper together with their proofs.

Theorem 2.1. *Let $G=(V,E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and average distance $\bar{l}$. Then*

$$\lambda_1 + \bar{l} \leq n$$

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

Proof. We always have that $\bar{l}(G) \leq \bar{l}(P_n) = \frac{n+1}{3} < \frac{n}{2}$, and so, if $\lambda_1 \leq \frac{n}{2}$, the proof is done. If $G \cong K_3$, the statement holds. Next, suppose that $n \geq 4$ and $\lambda_1 > \frac{n}{2}$. Stanley [26] proved that $\lambda_1 \leq \frac{-1+\sqrt{1+8m}}{2}$, from where it follows that

$$\frac{\lambda_1^2+\lambda_1}{2} \leq m. \tag{1}$$

Šoltés [25] proved that

$$\bar{l}(G) \leq \bar{l}(PK_{m,n}),$$

where $PK_{m,n}$ is the unique *path-complete graph* with m edges and n vertices, obtained from a clique and a path one end-vertex of which is adjacent to some vertices of the clique. The number k of vertices in a clique of $PK_{m,n}$ satisfies

$$\binom{k}{2} + (n-k) \leq m < \binom{k+1}{2} + (n-k-1). \tag{2}$$

From (1), (2) and $\lambda_1 > \frac{n}{2}$, we get that $k > \frac{n}{2} - 1$ and thus $n-k-1 < \frac{n}{2}$. Now, if $k \leq \lambda_1 - 1$, we have that

$$\binom{k+1}{2} + n - k - 1 \leq \frac{\lambda_1(\lambda_1-1)}{2} + \frac{n}{2} < \frac{\lambda_1(\lambda_1+1)}{2}$$

and we get a contradiction with (1) and (2). Thus, $k > \lambda_1 - 1$. Let $a = n-k$ be the number of vertices in a path of $PK_{m,n}$ and

$$k' = m - \binom{k}{2} - (n-k-1)$$

be the number of vertices in a complete subgraph adjacent to an end vertex of a path. From above, we have that

$$a < n - \lambda_1 + 1.$$

The average distance of $PK_{m,n}$ satisfies

$$\bar{l}(PK_{m,n}) = \frac{a+1}{3} \cdot \frac{\binom{a}{2}}{\binom{n}{2}} + 1 \cdot \frac{\binom{k}{2}}{\binom{n}{2}} + \frac{a+3}{2} \cdot \frac{ak}{\binom{n}{2}} - \frac{ak'}{\binom{n}{2}}.$$

Now, if $\lambda_1 \leq n-4$ it follows that $\frac{a+3}{2} \leq n-\lambda_1$, and thus $\bar{l}(G) \leq \frac{a+3}{2} \leq n-\lambda_1$. Next, suppose that $\lambda_1 > n-4$. Then $k > n-5$ and $a \leq 4$. If $a \in \{3,4\}$, then

$$\bar{l}(PK_{m,n}) \leq 1 \cdot \frac{\binom{k}{2}}{\binom{n}{2}} + \frac{a+3}{2} \cdot \frac{\binom{n}{2} - \binom{k}{2}}{\binom{n}{2}} = \frac{a+3}{2} - \frac{a+1}{2} \cdot \frac{\binom{k}{2}}{\binom{n}{2}}.$$

Hence $\bar{l}(PK_{m,n}) \leq a-1 < n-\lambda_1$ for $n \geq 8$ if $a=4$ and for $n \geq 11$ if $a=3$. The remaining cases are easily checked by hand.

If $a \in \{1,2\}$, then $\bar{l}(PK_{m,n}) < 1+\frac{6}{n}$. Thus, if $\lambda_1 \leq n-1-\frac{6}{n}$, the statement holds.

Next, suppose that $\lambda_1 > n-1-\frac{6}{n}$ and $a \in \{1,2\}$. From (1) it follows that $m > \binom{n}{2} - 6$, and thus, G misses at most five edges from a complete graph. If $n \leq 10$, the corresponding cases are easily checked by hand. If $n \geq 11$, then there exists a vertex adjacent to all other vertices of G, and thus

$$\bar{l}(G) = 1 \cdot \frac{m}{\binom{n}{2}} + 2 \cdot \frac{\binom{n}{2} - m}{\binom{n}{2}} \leq 1 + \frac{10}{n(n-1)}.$$

However, since $G \ncong K_n$, we have that G is a subgraph of $K_n - e$ and thus

$$\lambda_1 \leq \lambda_1(K_n - e) = \frac{n-3+\sqrt{n^2+2n-7}}{2} < n-1-\frac{2}{n+1},$$

from where we see that the statement holds.

Finally, if $a=0$, then $G \cong K_n$, and the statement holds. ■

Contrary to the case of the upper bound, AGX 2 was not able to make any conjecture for the lower bound on $\lambda_1 + \bar{l}$, since, at least at first sight, it appears that there is no common structure for the extremal graphs found. A few of these extremal graphs are given in Figure 1.

The following result was derived for a structural result of AGX 2.

Theorem 2.2. *Let $G=(V,E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and independence number α. Then*

$$\alpha + \lambda_1 \leq \frac{n+\alpha'-1+\sqrt{(n-\alpha'-1)^2+4\alpha'(n-\alpha')}}{2}, \tag{3}$$

with equality if and only if G is the complete split graph $S_{n,\alpha'}$, where α' is given by

$$\alpha' = \begin{cases} \left\lfloor \frac{n+1+\sqrt{n^2-n+1}}{3} \right\rfloor & \text{for } n=3k \text{ or } n=3k+2, \\ \left\lceil \frac{n+1+\sqrt{n^2-n+1}}{3} \right\rceil & \text{for } n=3k+1. \end{cases}$$

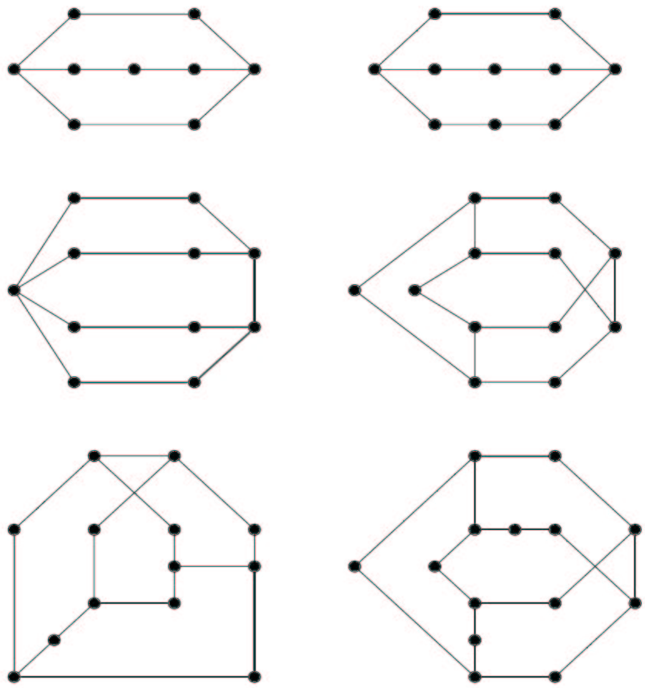

Figure 1. Graphs likely to minimize $\lambda_1 + \bar{l}$ for $n = 9, \ldots, 14$.

Proof. For a fixed independence number α, every graph with n vertices and independence number α is a subgraph of a complete split graph $S_{n,\alpha}$. Then, since the index of a graph increases by adding edges, we see that the graph maximizing the index λ_1 is $S_{n,\alpha}$. Thus, in order to prove our theorem, we have to find out for which α the complete split graph $S_{n,\alpha}$ has the largest sum $\alpha + \lambda_1$. Let us consider the matrix M associated to the divisor (cf. Chapter 4 of [9]) of a complete split graph $S_{n,\alpha}$

$$M = \begin{pmatrix} n-\alpha-1 & \alpha \\ n-\alpha & 0 \end{pmatrix}.$$

The index of $S_{n,\alpha}$ is exactly the largest eigenvalue of M, which is

$$\lambda_1 = \frac{n-\alpha-1+\sqrt{(n-\alpha-1)^2+4\alpha(n-\alpha)}}{2}.$$

Thus, in $S_{n,\alpha}$ we have

$$\alpha + \lambda_1 = f(n, \alpha) = \frac{n + \alpha - 1 + \sqrt{(n - \alpha - 1)^2 + 4\alpha(n - \alpha)}}{2}.$$

Provided that

$$n - 3\alpha + 1 < 0, \tag{4}$$

the stationary point is at

$$\alpha' = \frac{n + 1 + \sqrt{n^2 - n + 1}}{3},$$

which is between $\frac{4n+1}{6}$ and $\frac{4n+2}{6}$. However, since α' in a complete split graph must be an integer, the extremal graph is obtained for α' equal to one of $\left\lfloor \frac{n+1+\sqrt{n^2-n+1}}{3} \right\rfloor$ and $\left\lceil \frac{n+1+\sqrt{n^2-n+1}}{3} \right\rceil$. Straightforward but tedious analysis, divided in cases according to the remainder of n modulo 3, shows which of the two possible values for α' gives the extremal graph.

What if (4) does not hold? In that case $\alpha \le \frac{n+1}{3}$. If $\alpha = 1$, then $\lambda_1 = n - 1$ and $\alpha + \lambda_1 = n$. Otherwise, for $\alpha \ge 2$ we have $\lambda_1 < n - 1$ and

$$\alpha + \lambda_1 < \frac{4n - 2}{3},$$

which is less than $f(n, \alpha')$, so no other extremal graph may exist in this case. ■

Let $PV(G)$ be a graph obtained by adding a pendant vertex to each vertex of a graph G. Concerning $\lambda_1 - \beta$, we are able to prove the following relation, derived from a structural result of AGX 2.

Theorem 2.3. *Let $G = (V, E)$ be a connected graph of even order $n \ge 2$ with index λ_1 and domination number β. Then*

$$\lambda_1 - \beta \ge \cos\frac{2\pi}{n+1} + \sqrt{1 + \cos^2\frac{2\pi}{n+1}} - \frac{n}{2}. \tag{5}$$

with equality if and only if G is a caterpillar $PV(P_{n/2})$.

Proof. Let $n = 2k$. We consider two cases. First, suppose that $\beta = k$. Deletion of an edge from a connected graph decreases the index and does not decrease the domination number. Thus, if G is not a tree, the value of $\lambda_1 - \beta$ is smaller for any spanning tree of G. So, we may suppose that G is indeed a tree.

To prove this theorem, we need some intermediate results. First, note that the following lemma can also be found in [12].

Lemma 2.4. *Let T be a tree with $2k$ vertices and $\beta = k$, $k \geq 1$. Then there exists a tree T' with k vertices such that $T = PV(T')$.*

***Proof of Lemma* 2.4.** The proof is by induction. If $k = 1$, then $T \cong K_2$ and $T' \cong K_1$.

Suppose that the statement holds for all trees with less than $2k$ vertices, and let T be a tree with $2k$ vertices and $\beta = k$. We may assume that a dominating set S of size β in T does not contain pendant vertices: indeed, if any such vertex is replaced by its neighbor, the resulting set is still dominating. Let u be a pendant vertex of T with v as its unique neighbor. By our assumption, $v \in S$.

We show that u is the unique pendant vertex adjacent to v. Otherwise, let U, $|U| \geq 2$, be the set of all pendant vertices adjacent to v, and let S' be the minimum dominating set of $T - (\{v\} \cup U)$. According to Ore [23], a complement of a minimal dominating set is a dominating set. It follows that

$$|S'| \leq k - \frac{1 + |U|}{2}.$$

Then $S' \cup \{v\}$ is a dominating set of T of size less than k, which is a contradiction.

Next, the set $S \setminus \{v\}$ is a minimum dominating set in $T - \{u, v\}$. By the induction hypothesis, there exists a tree T'' such that $T - \{u, v\} = PV(T'')$. The tree T' is then obtained by adding v to T'' and joining it to its non-pendant neighbors in T, which are already contained in T''.

Lemma 2.5. *Let G be a graph with eigenvalues λ_i, $i = 1, 2, \ldots, k$. The eigenvalues of $PV(G)$ have the form*

$$\frac{1}{2}\left(\lambda_i \pm \sqrt{4 + \lambda_i^2}\right), \quad i = 1, 2, \ldots, k.$$

***Proof of Lemma* 2.5.** Denote by v_i, $i = 1, 2, \ldots, k$, the vertices of G, and by v_i' the pendant vertex attached to v_i in $PV(G)$. Let λ be a nonzero eigenvalue of $PV(G)$ with a corresponding eigenvector x, and to simplify notation, let $x_i = x_{v_i}$ and $x'_i = x_{v'_i}$. From the eigenvalue equation at v'_i, we have

$$\lambda x'_i = x_i,$$

or $x'_i = \frac{1}{\lambda} x_i$. Next, at v_i we have

$$\lambda x_i = x'_i + \sum_{v_j \sim v_i} x_j,$$

(where $v_j \sim v_i$ denotes the fact that v_j is a neighbor of v_i) from where it follows that

$$\left(\lambda - \frac{1}{\lambda}\right) x_i = \sum_{v_j \sim v_i} x_j.$$

The last relation shows that the vector $(x_i)_{i=1}^k$ is an eigenvector of G corresponding to the eigenvalue $\lambda - \frac{1}{\lambda}$.

Next, for every i, $1 \leq i \leq k$, the equation

$$\lambda - \frac{1}{\lambda} = \lambda_i$$

has two real nonzero solutions equal to

$$\lambda = \frac{1}{2}\left(\lambda_i \pm \sqrt{4 + \lambda_i^2}\right).$$

Both of these solutions are eigenvalues of $PV(G)$, as the eigenvector x of G corresponding to λ_i may be extended to an eigenvector of $PV(G)$ by setting $x'_j = \frac{1}{\lambda} x_j$ for every pendant vertex v'_j. As this process provides us with a set of $2k$ independent eigenvectors of $PV(G)$, we conclude that there are no further eigenvalues of $PV(G)$ (and, in fact, zero may not be an eigenvalue of $PV(G)$).

Since $\lambda_1 \geq |\lambda_i|$ for $i = 2, \ldots, k$, we obtain from Lemma 2.5 that the index of $PV(G)$ is equal to

$$\frac{1}{2}\left(\lambda_1(G) + \sqrt{4 + \lambda_1^2(G)}\right).$$

Now, the path P_k has the minimum index among trees with k vertices. Based on the previous lemmas, we may conclude that $PV(P_k)$ has the minimum index among trees with $2k$ vertices and domination number $\beta = k$. Since the index of P_k is equal to $2\cos\frac{2\pi}{k+1}$, from Lemma 2.5 we see that the index of $PV(P_k)$ is equal to

$$\cos\frac{2\pi}{k+1} + \sqrt{1+\cos^2\frac{2\pi}{k+1}},$$

and the theorem follows.

For the remaining case, suppose that $\beta < k$. Then $\beta \leq k-1$. Graph G is connected and has at least three vertices, and thus contains a star $K_{1,2}$ or a triangle K_3 as an induced subgraph. From the Interlacing Theorem [9, p. 19] we have that $\lambda_1(G) \geq \sqrt{2}$. Together, this implies that

$$\lambda_1 - \beta \geq 1 + \sqrt{2} - \frac{n}{2} > \cos\frac{2\pi}{k+1} + \sqrt{1+\cos^2\frac{2\pi}{k+1}} - \frac{n}{2},$$

showing that (5) is true and that there are no new extremal graphs in this case. ■

3. A Few Propositions

A number of conjectures turn out to be true and novel, but with a proof that is considerably easier to find than in the case of the previous three theorems. Such results are next given, in subsections corresponding to each invariant.

3.1. The chromatic number

Proposition 3.1. *Let G be a connected graph on $n \geq 3$ vertices with index λ_1 and chromatic number χ. Then*

$$\frac{\lambda_1}{\chi} \geq \frac{2}{3}$$

with equality if and only if G is an odd cycle C_n. Moreover, if n is even, the inequality is strict and the minimum value of λ_1/χ is attained for a short lollipop SL_n.

Proof. The proof is divided in cases based on the value of χ:

- $\chi = 2$. It is known that for a connected graph, the path P_n has a minimum index equal to $2\cos\frac{\pi}{n+1}$ (see [21] or [9, p. 78]). Since $n \geq 3$, we have that

$$\frac{\lambda_1}{\chi} \geq \cos\frac{\pi}{n+1} \geq \frac{\sqrt{2}}{2} > \frac{2}{3}.$$

- $\chi \geq 3$. According to Wilf [27], $\lambda_1 \geq \chi - 1$. So

$$\frac{\lambda_1}{\chi} \geq \frac{\chi-1}{\chi} \geq \frac{2}{3}$$

with equality if and only if $\lambda_1 = 2$ and $\chi = 3$ and then G is an odd cycle. If n is even and since $\chi \geq 3$, G is not a cycle but contains an odd cycle C_k and then a short lollipop SL_k. Since λ_1 decreases by deleting an edge from a connected graph, we can delete edges until we are left with a short lollipop SL_k. Thus

$$\lambda_1(G) \geq \lambda_1(SL_k) \geq \lambda_1(SL_n) > \tau^{1/2} + \tau^{-1/2},$$

where $\tau = \frac{1+\sqrt{5}}{2}$ (for the last two inequalities above, see [18, p. 169]). The minimum value of $\frac{\lambda_1}{\chi}$ is attained if and only if $G \cong SL_n$. ■

Very recently Feng, Li and Zhang [13] characterized graphs with given χ and minimum or maximum λ_1. These results could lead to an alternate proof of Proposition 3.1.

Proposition 3.2. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and chromatic number χ. Then*

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

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

Proof. Since the addition of an edge to a connected graph increases λ_1 (see, e.g., [9, p. 19]), for a constant value of χ the maximal value of $\frac{\lambda_1}{\chi}$ is attained for a complete χ-partite graph. Again, we divide the proof into cases based on the value of χ:

- $\chi = 2$. Hong [20] proved that, among bipartite graphs, the complete balanced bipartite graph has maximum index, equal to $\sqrt{\lfloor n/2\rfloor \cdot \lceil n/2\rceil}$. Thus, the theorem follows in this case.

- $\chi \geq 3$. According to [9, p. 92], for a χ-partite graph

$$\lambda_1 \leq \frac{\chi - 1}{\chi} n.$$

Then

$$\frac{\lambda_1}{\chi} \leq \frac{\chi - 1}{\chi^2} n \leq \frac{2n}{9} < \frac{1}{2}\sqrt{\left\lfloor \frac{n}{2} \right\rfloor \cdot \left\lceil \frac{n}{2} \right\rceil}.$$

This complete the proof. ∎

3.2. The maximum degree

Proposition 3.3. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and maximum degree Δ. Then*

$$\lambda_1 - \Delta \geq \sqrt{n-1} - n + 1.$$

The equality is attained for a star S_n.

Proof. A connected graph G contains a spanning tree T with the same maximum degree Δ. Deleting from G edges that are not in T, the index decreases. Further, since T contains a star $K_{1,\Delta}$, its index is at least $\sqrt{\Delta}$, with equality if and only if $T \cong K_{1,\Delta}$. Therefore, we have that

$$f(\Delta) = \sqrt{\Delta} - \Delta \leq \lambda_1 - \Delta.$$

The function $f(\Delta)$ is decreasing in $[1, n-1]$, and its minimum is attained for $\Delta = n - 1$, which proves the inequality.

The equality is attained if and only if $G \cong T$, $T \cong K_{1,\Delta}$ and $\Delta = n - 1$, i.e., if and only if $G \cong K_{1,n-1}$. ∎

Using a similar argument, one can also prove the following

Proposition 3.4. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and maximum degree Δ. Then*

$$\frac{\lambda_1}{\Delta} \geq \frac{1}{\sqrt{n-1}}.$$

The equality is attained for a star S_n.

3.3. The minimum degree

Proposition 3.5. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and minimum degree δ. Then*

$$\lambda_1 - \delta \leq n - 3 + \varepsilon,$$

where ε is the root of

$$\varepsilon^3 + (2n-3)\varepsilon^2 + (n^2 - 3n + 1)\varepsilon - 1 = 0,$$

satisfying $0 < \varepsilon < 1$. The equality is attained for a short kite SK_n.

Proof. Let H_δ be a graph obtained from a clique on $n-1$ vertices by adding a vertex adjacent to δ vertices in the clique. If u is a vertex of degree δ in G, then by adding edges between any two vertices in $G - u$, we get a graph isomorphic to H_δ, showing that

$$\lambda_1(G) - \delta \leq \lambda_1(H_\delta) - \delta.$$

Rowlinson [24] proved that

$$\lambda_1(H_\delta) = n - 2 + \varepsilon_\delta,$$

where $0 < \varepsilon_\delta < 1$ and ε_δ is the solution of

$$\varepsilon^3 + (2n-3)\varepsilon^2 + (n^2 - 3n + 2 - \delta)\varepsilon - \delta^2 = 0.$$

We show that $\lambda_1(H_\delta) - \delta$ strictly decreases when δ increases. This follows from

$$\begin{aligned} &\big(\lambda_1(H_\delta) - \delta\big) - \big(\lambda_1(H_{\delta+1}) - (\delta+1)\big) \\ &= (n - \delta - 2 + \varepsilon_\delta) - (n - \delta - 3 + \varepsilon_{\delta+1}) = 1 + (\varepsilon_\delta - \varepsilon_{\delta+1}) > 0. \end{aligned}$$

Thus, the maximum of $\lambda_1(H_\delta) - \delta$ is attained for $\delta = 1$, and the inequality in the proposition follows.

The equality is attained if and only if $G \cong H_\delta$ for $\delta = 1$, i.e., for and only for the short kite SK_n. ■

Using a similar argument, one can also prove the following relation derived from a structural result of AGX 2.

Proposition 3.6. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and minimum degree δ. Then*

$$\frac{\lambda_1}{\delta} \leq n - 2 + \varepsilon$$

where ε is the root of

$$\varepsilon^3 + (2n-3)\varepsilon^2 + (n^2 - 3n + 1)\varepsilon - 1 = 0,$$

satisfying $0 < \varepsilon < 1$. The equality is attained for a short kite SK_n.

3.4. The average degree

Proposition 3.7. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and average degree $\bar{d}$. Then*

$$\frac{\lambda_1}{\bar{d}} \leq \frac{n}{2\sqrt{n-1}}.$$

The equality is attained for a star S_n.

Proof. Using $\bar{d} = \frac{2m}{n}$ and the upper bound $\lambda_1 \leq \sqrt{2m - n + 1}$ (see [19]), we have

$$\frac{\lambda_1}{\bar{d}} = \frac{n\lambda_1}{2m} \leq \frac{n\sqrt{2m-n+1}}{2m}.$$

Denoting the right-hand side of the above inequality by a function $f(m)$ in m and derivating gives

$$f'(m) = \frac{n(n-1-m)}{2m^2\sqrt{2m-n+1}},$$

showing that the function f is decreasing for $m \geq n-1$, which is also the minimum number of edges a connected graph may have. Thus, the maximum of $f(m)$ is reached for $m = n-1$, and the inequality in the proposition follows.

The equality is attained if and only if $m = n-1$ and $\lambda_1 = \sqrt{n-1}$, which happens only for a star S_n. ■

3.5. The radius

Proposition 3.8. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and radius r. Then*

$$\lambda_1 + r \leq n.$$

The equality is attained for the complete graph K_n or the complement of a matching $\overline{\frac{n}{2}K_2}$.

Proof. It is known that [9] $\lambda_1 \leq \Delta$ with equality if and only if G is regular. Thus to prove the bound, it suffices to show that $\Delta + r \leq n$ and then characterize the extremal graphs.

If $r = 1$, then $\Delta = n - 1$, and $\Delta + r = n$. The equality in $\lambda_1 + r \leq n$ now holds if and only if $\lambda_1 = n - 1$, i.e., G is the complete graph.

If $r = 2$, from the ineqaulity (see [6])

$$r \leq \frac{n - \Delta + 2}{2}, \tag{6}$$

it follows that $\Delta + r + 2 = \Delta + 2r \leq n + 2$. Hence $\Delta + r \leq n$, with equality if and only if $\Delta = n - 2$. The equality in $\lambda_1 + r \leq n$ now holds if and only if G is regular of degree $n - 2$, i.e., G is a complement of a matching.

If $r \geq 3$, using again inequality (6), we have $\Delta + r + 3 \leq \Delta + 2r \leq n + 2$, and so $\Delta + r < n$. Hence, the equality is never attained in this case. ■

3.6. The domination number

Proposition 3.9. *Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and domination number β. Then*

$$\lambda_1 + \beta \leq n.$$

The equality is attained for the complete graph K_n or a complement of the matching $\overline{\frac{n}{2}K_2}$.

Proof. Let u be a vertex of maximum degree Δ in $G = (V, E)$. The set $S_u = V \setminus N[u]$, where $N[u] = \{u\} \cup N(u)$ and $N(u)$ is the set of all neighbors of u, is a dominating set of size $n - \Delta$. Thus, $\beta \leq n - \Delta$.

On the other hand, it is well known that $\lambda_1 \leq \Delta$ (see, e.g., [9]).

Thus

$$\lambda_1 + \beta \leq \Delta + (n - \Delta) = n.$$

The equality is attained if both $\beta = n - \Delta$ and $\lambda_1 = \Delta$. The latter equality holds if and only if G is a Δ-regular graph. Then the former equality holds if and only if S_u is a minimum dominating set for every vertex u of G. In particular, this yields that there are no edges in a graph induced by non-neighbors of u. If $\Delta = n - 1$, then there are no non-neighbors of u and $G \cong K_n$. If $\Delta < n - 1$, then for each non-neighbor $v \notin N[u]$ one has $N(v) = N(u)$, as v may be adjacent only to neighbors of u and, since G is regular, v has to be adjacent to all neighbors of u. Now, a minimum dominating set may be obtained by taking vertex u and one of its neighbors, showing that $\beta = 2$ and, as a consequence from $\beta = n - \Delta$, that $\Delta = n - 2$. Thus, in this case it follows that $G \cong \overline{\frac{n}{2}K_2}$. ■

4. CONJECTURES AND REFUTATIONS

4.1. Open conjectures

When it comes to proving them, conjectures obtained with AGX 2 are very varied. We next list a few conjectures for which we were unable to find a proof (or a counterexample), and which we find interesting.

Conjecture 4.1. Among all connected graphs on n vertices, the maximum value of $\lambda_1 - \bar{d}$ is attained for a pineapple graph $PA_{n,k}$ with $1 \leq k \leq n - 1$.

This conjecture is discussed in more detail in [4].

The following three conjectures may be approached using the results of [17]. It is proved there that among graphs with n vertices and diameter $D \geq 2$, the maximum index is attained by a balanced bug $Bug_{n-D+2,\lceil D/2\rceil,\lfloor D/2\rfloor}$ when $D \geq 2$. Similarly, among all graphs with n vertices and radius $r \geq 3$, the maximum index is attained by an odd bag $Bag_{n-2r+3,2r-1}$. Thus, in each of the following conjectures we know that the extremal graph must be either a bag or a bug, but, at the moment we are not able to prove exactly which bag or bug, as we cannot approximate their index well enough.

Conjecture 4.2. Let $G = (V, E)$ be a connected graph on $n \geq 2$ vertices with index λ_1 and diameter D. Then

$$\lambda_1 + D \leq n - 1 + 2\cos\frac{\pi}{n+1}.$$

The inequality is sharp for and only for paths.

Conjecture 4.3. The maximum value of $\lambda_1 \cdot D$ is obtained for a balanced bug $Bug_{\lfloor n/2 \rfloor+2,\lceil n/4 \rceil,\lfloor (n+1)/4 \rfloor}$.

Conjecture 4.4. The maximum value of $\lambda_1 \cdot r$ is obtained for a $Bag_{\lfloor n/2 \rfloor+2,\lceil n/2 \rceil}$.

4.2. Counterexamples

We will now comment on the refuted conjectures. The role of counterexamples, especially those that appear repeatedly, is to equip the mathematician with an arsenal of graphs which he or she may use to test every new conjecture in order to gain initial insight into its behaviour. Here, we give a sample of counterexamples for the refuted conjectures.

First, the conjectures on the lower bounds for the expressions

$$\lambda_1 + D, \quad \lambda_1 \cdot D, \quad \lambda_1 + r \quad \text{and} \quad \lambda_1 \cdot r$$

are all refuted by the same well-known family of graphs: the cubes. Namely, the m-dimensional cube Q_m has $n = 2^m$ vertices, it is m-regular implying that $\lambda_1(Q_m) = m$, and both its diameter and radius are also equal to m. Thus, the above expressions for Q_m have the value either $2m$ or m^2. On the other hand, all conjectured lower bounds contain the factor or summand $\sqrt{n-1} = \sqrt{2^m - 1}$, which is exponential in m and becomes larger than both $2m$ and m^2 for m large enough (actually, for $m \geq 17$).

Next, the conjecture on the upper bound for $\lambda_1 \cdot \bar{l}$ is false. AGX 2 conjectured that the extremal graph is $K_n - e$ for every n. While $K_n - e$ has λ_1 close to the maximum value of $n-1$, its average distance is barely larger than the minimum value of 1. Thus, a graph which has λ_1 and $\bar{l}$ closer to each other may have larger value of the product $\lambda_1 \cdot \bar{l}$. It is easy to get to such a graph: if we want to have large λ_1, it is sufficient to have a big clique in it; if want to have large $\bar{l}$, it is sufficient to have a long induced path. Thus, a natural candidate for a counterexample is a graph $KP_{p,q}$ consisting of a complete graph K_p and a path P_q, in which one end-vertex of a path is adjacent to a vertex of a complete graph (in other words $K_{p,q}$ is a kite). A small counterexample is indeed obtained already for $p = q = 4$.

The situation is similar with the lower bound for $\lambda_1 + \beta$. The conjectured extremal graphs are stars which have the smallest possible domination number β, while the index is far from the minimum value: every tree on n vertices has index at most $\sqrt{n-1}$. Thus, it appears to be appropriate to look for a counterexample among trees with higher domination number. Even $\beta = 2$ suffices: a tree consisting of two copies of a star S_8 and another vertex adjacent to a center of each star has $n = 19$ vertices and $\lambda_1 \approx 3.16228$, giving a small counterexample. In general, forming a tree by taking a path of length 2β and attaching k pendant vertices at every odd vertex of this path creates a tree with $n = 1 + \beta(k+2)$ vertices, the domination number β and the index λ_1 approximately equal to $\sqrt{\frac{n}{\beta}}$, yielding the sum $\lambda_1 + \beta$ of order $\sqrt{\frac{n}{\beta}} + \beta$, which is less than $1 + \sqrt{n-1}$ for β large enough.

5. Conclusion

Using AGX, the index of a connected graph G has been compared with the chromatic number χ, the largest degree Δ, the smallest degree δ, the average degree $\bar{d}$, the diameter D, the radius r, the average distance $\bar{l}$ between pairs of distinct vertices, the independence number α and the domination number β, looking for upper and lower bounds which are functions of the order of G.

There are 72 cases altogether: in 7 cases known results were reproduced, in 32 cases immediate results were obtained and automatically proved by the system, conjectures were obtained in 27 cases, of which 12 were proved (in 3 theorems and 9 propositions), 9 remain open and 6 were refuted. No results could be derived in 7 cases.

Appendix

We give full details of all 72 cases examined with AGX 2 in Table 1. Each expression of the form $\lambda_1 * i(G)$ occupies one row of the table, and the expression itself is given in the first column. Each expression yields two cases, the first one concerning its lower bound and the second its upper bound. Each of these cases occupies three columns which contain:

- a formula giving the value of the bound, if known;
- the status of the conjecture, which is one of the following: immediate, refuted, known, proved (with reference to a theorem or proposition in this article), open or no result.
- the family of extremal graphs.

If a cell of the table is empty, it means that we do not know its contents.

Table 1. Details of conjectures obtained with AGX 2.

$i_1 * i_2$	bound	status	extremal graphs
$\lambda_1 - \chi \ \geq$	-1	known	$\overline{K_n}$; C_n for odd n
$\lambda_1 - \chi \leq$		open	$\overline{K_{p_1,\cdots p_{\lceil\sqrt{n}\rceil}}}$, $(\forall i,j)\,\lvert p_i - p_j\rvert \leq 1$
$\lambda_1 + \chi \geq$	$2 + 2cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 + \chi \leq$	$2n-1$	immediate	K_n
$\lambda_1/\chi \geq$	$\frac{2}{\sqrt{\lfloor\frac{n}{2}\rfloor\cdot\lceil\frac{n}{2}\rceil}}$	Prop. 3.2	$K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$
$\lambda_1/\chi \leq$	$\frac{2}{3}$	Prop. 3.1	C_n for odd n, SL_n for even n
$\lambda_1 \cdot \chi \geq$	$4cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 \cdot \chi \leq$	$n(n-1)$	immediate	K_n
$\lambda_1 - \Delta \geq$	$\sqrt{n-1} - n + 1$	Prop. 3.3	S_n
$\lambda_1 - \Delta \leq$	0	known	regular graphs
$\lambda_1 + \Delta \geq$	$2 + 2cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 + \Delta \leq$	$2n-2$	immediate	K_n
$\lambda_1/\Delta \geq$	$\frac{1}{\sqrt{n-1}}$	Prop. 3.4	S_n
$\lambda_1/\Delta \leq$	1	known	regular graphs
$\lambda_1 \cdot \Delta \geq$	$4cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 \cdot \Delta \leq$	$(n-1)^2$	immediate	K_n
$\lambda_1 - \delta \geq$	0	known	regular graphs
$\lambda_1 - \delta \leq$	$n - 3 + \varepsilon$	Prop. 3.5	SK_n
$\lambda_1 + \delta \geq$	$1 + 2\cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 + \delta \leq$	$2n-2$	immediate	K_n
$\lambda_1/\delta \geq$	1	known	regular graphs
$\lambda_1/\delta \leq$	$n - 2 + \varepsilon$	Prop. 3.6	SK_n
$\lambda_1 \cdot \delta \geq$	$2\cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 \cdot \delta \leq$	$(n-1)^2$	immediate	K_n
$\lambda_1 - \overline{d} \geq$	0	known	regular graphs
$\lambda_1 - \overline{d} \leq$		open	$PA_{n,k}$
$\lambda_1 + \overline{d} \geq$	$2 - \frac{2}{n} + 2\cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 + \overline{d} \leq$	$2n-2$	immediate	K_n
$\lambda_1/\overline{d} \geq$	1	known	regular graphs
$\lambda_1/\overline{d} \leq$	$\frac{n}{2\sqrt{n-1}}$	Prop. 3.7	S_n
$\lambda_1 \cdot \overline{d} \geq$	$(4 - \frac{4}{n})\cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1 \cdot \overline{d} \leq$	$(n-1)^2$	immediate	K_n
$\lambda_1 - D \geq$	$2\cos\frac{\pi}{n+1} - n + 1$	immediate	P_n
$\lambda_1 - D \leq$	$n-2$	immediate	K_n
$\lambda_1 + D \geq$	$2 + \sqrt{n-1}$	refuted	S_n
$\lambda_1 + D \leq$	$n - 1 + 2\cos\frac{\pi}{n+1}$	open	P_n
$\lambda_1/D \geq$	$\frac{2}{n-1}\cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1/D \leq$	$n-1$	immediate	K_n
$\lambda_1 \cdot D \geq$	$2\sqrt{n-1}$	refuted	S_n
$\lambda_1 \cdot D \leq$		open	$Bug_{\lfloor n/2\rfloor+2,\lceil n/4\rceil,\lfloor(n+1)/4\rfloor}$
$\lambda_1 - r \geq$	$2\cos\frac{\pi}{n+1} - \lfloor\frac{n}{2}\rfloor$	immediate	P_n
$\lambda_1 - r \leq$	$n-2$	immediate	K_n
$\lambda_1 + r \geq$	$1 + \sqrt{n-1}$	refuted	S_n
$\lambda_1 + r \leq$	n	Prop. 3.8	K_n; $\overline{\frac{n}{2}K_2}$ for even n
$\lambda_1/r \geq$	$\frac{2}{\lfloor n/2\rfloor}\cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1/r \leq$	$n-1$	immediate	K_n

Table 1 – continued from previous page

$\lambda_1 \cdot r \geq$	$\sqrt{n-1}$	refuted	S_n
$\lambda_1 \cdot r \leq$		open	$Bag_{\lfloor n/2\rfloor+2,\lceil n/2\rceil}$
$\lambda_1 - \bar{l} \geq$	$2\cos\frac{\pi}{n+1} - \frac{n+1}{3}$	immediate	P_n
$\lambda_1 - \bar{l} \leq$	$n-2$	immediate	K_n
$\lambda_1 + \bar{l} \geq$		open	
$\lambda_1 + \bar{l} \leq$	n	Theorem 2.1	K_n
$\lambda_1/\bar{l} \geq$	$\frac{6}{n+1}\cos\frac{\pi}{n+1}$	immediate	P_n
$\lambda_1/\bar{l} \leq$	$n-1$	immediate	K_n
$\lambda_1 \cdot \bar{l} \geq$		no result	
$\lambda_1 \cdot \bar{l} \leq$	$\frac{n^2-n+2}{2n(n-1)}\left(n-3+\sqrt{n^2+2n-7}\right)$	refuted	$K_n - e$
$\lambda_1 - \alpha \geq$	$\sqrt{n-1} - n + 1$	open	S_n
$\lambda_1 - \alpha \leq$	$n-2$	immediate	K_n
$\lambda_1 + \alpha \geq$		no result	
$\lambda_1 + \alpha \leq$	$\frac{2n-1+2\sqrt{n^2-n+1}}{3}$	Theorem 2.2	$S_{n,\alpha}$
$\lambda_1/\alpha \geq$		no result	
$\lambda_1/\alpha \leq$	$n-1$	immediate	K_n
$\lambda_1 \cdot \alpha \geq$		open	connected Turan graph
$\lambda_1 \cdot \alpha \leq$		no result	
$\lambda_1 - \beta \geq$		Theorem 2.3	caterpillars, $\beta = \lceil n/2\rceil$
$\lambda_1 - \beta \leq$	$n-2$	immediate	K_n
$\lambda_1 + \beta \geq$	$1+\sqrt{n-1}$	refuted	S_n
$\lambda_1 + \beta \leq$	n	Prop. 3.9	K_n; $\overline{\frac{n}{2}K_2}$ for even n
$\lambda_1/\beta \geq$	$\frac{1}{n-1}$	immediate	K_n
$\lambda_1/\beta \leq$		no result	
$\lambda_1 \cdot \beta \geq$		open	connected Turan graph
$\lambda_1 \cdot \beta \leq$		no result	

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Received 23 July 2007
Revised 16 October 2008
Accepted 16 October 2008