Variable Neighborhood Search for Extremal Graphs, 16. Some Conjectures Related to the Largest Eigenvalue of a Graph

Aouchiche M., Bell F.K., Cvetković D., Hansen P., Rowlinson P., Simić S., Stevanović D.

Abstract. We consider four conjectures related to the largest eigenvalue of (the adjacency matrix of) a graph (i.e., to the index of the graph). Three of them have been formulated after some experiments with the programming system AutoGraphiX (AGX), designed for finding extremal graphs with respect to given properties by the use of variable neighborhood search. The conjectures are related to the maximal value of the irregularity and spectral spread in \( n \)-vertex graphs, to a Nordhaus-Gaddum type upper bound for the index, and to the maximal value of the index for graphs with given numbers of vertices and edges. None of the conjectures has been resolved so far. We present partial results and provide some indications that the conjectures are very hard.

Key words and phrases: metaheuristics, combinatorial optimization, variable neighborhood search, extremal graph theory, graph spectra, largest eigenvalue

1 Introduction

The variable neighborhood search appears to play a specific role in connections and interactions between combinatorial optimization and extremal graph theory.

Combinatorial optimization (Mathematics Subject Classification: 90C27) deals with solving optimization problems of the following type

\[
\min_{x \in S} f(x)
\]

where \( S \) is a finite or infinite denumerable set and \( f : S \to \mathbb{R} \). In most cases the set of feasible solutions \( S \) is a finite set.

Extremal graph theory (Mathematics Subject Classification: 05C35) deals with finding (lower and/or upper) bounds for various graph invariants under some constraints imposed on other graph invariants (Bollobás 1978; Bollobás 1995). Construction of extremal graphs, i.e., graphs meeting these bounds is a natural part of such investigations.

The key observation of Cvetković et al. (2004) is that the unifying feature of these two disciplines is the fact that both deal with problems of finding extrema of a real function defined on a finite set.

There are many problems in (extremal) graph theory where one looks for extrema of a graph invariant for graphs with a fixed number of vertices. Such a problem can be represented in the form of (1) where \( S \) is the set of all (or some) graphs on a fixed number of vertices and for a graph \( x \in S \) the function \( f(x) \)
is a graph invariant. Such a problem was recognized as a generic problem of combinatorial optimization for the first time in (Caporossi and Hansen 2000).

A computer program called AutoGraphiX (AGX), for finding extremal (or near-extremal) graphs with respect to some properties, has been described in (Caporossi and Hansen 2000). The paper was just the beginning of a series of papers in which results obtained by AGX are presented. To this series belong the papers (Caporossi and Hansen 2000; Caporossi et al. 1999a; Cvetković et al. 2001; Caporossi et al. 1999b; Caporossi and Hansen 2004; Hansen and Mélot 2003; Fowler et al. 2001; Aouchiche et al. 2001; Hansen and Mélot 2005; Gutman et al. 2005; Aouchiche et al. 2005; Aouchiche and Hansen; Belhaïza et al. 2005; Hansen et al. 2005; Hansen and Stevanović) (and this paper as well).

As one of the first test examples, the following extremal problem with previously known solution was tested by AGX (Caporossi and Hansen 2000). Let \( T_n \) be the set of trees on \( n \) vertices and let \( \lambda_1(G) \) be the largest eigenvalue of the adjacency matrix of a graph \( G \). Find

\[
\min_{T \in T_n} \lambda_1(T), \quad \max_{T \in T_n} \lambda_1(T).
\]

and the corresponding extremal trees. As is well known, the minimum is attained for a path \( P_n \) with \( \lambda_1(P_n) = 2 \cos \frac{\pi}{n+1} \) and the maximum for a star \( K_{1,n-1} \) with \( \lambda_1(K_{1,n-1}) = \sqrt{n-1} \) (Lovász and Pelikan 1973). The system AGX has successfully found these extremal trees for several values of \( n \) (Caporossi and Hansen 2000). Obviously, problems (2) are of the form (1).

Combinatorial optimization and extremal graph theory existed for many years without notable interactions. For example, the books (Bollobás 1978; Bollobás 1995) on extremal graph theory do not refer to combinatorial optimization.

Recently, the idea was built into the system AGX (Caporossi and Hansen 2000) and the application of this system to actual research on extremal problems in graph theory clearly indicates a possibility of connecting the two fields. Some general solving procedures of combinatorial optimization can be used via programming systems, such as AGX, to solve problems of extremal graph theory in order to give hints concerning theoretical considerations. In particular, variable neighborhood search is used as the main (meta-)heuristic within the system AGX.

For example, in (Cvetković et al. 2001) the system AGX has found extremal spanning trees of a complete bipartite graph \( K_{m,n} \) for various \( m \) and \( n \) w.r.t. the objective function \( \lambda_1(T) \). Many conjectures arose and some of them have been proved in (Cvetković et al. 2001).

In this paper we consider four conjectures related to the index of a graph. Three of them have been formulated after some experiments with the system AGX. The conjectures appear to be very challenging and none of them has been resolved so far. We present partial results and provide some indications that the conjectures are very hard.

Section 2 contains some necessary definitions. In Section 3 the three conjectures related to AGX are formulated, while the fourth conjecture is given
in Section 4. We start in Section 5 presenting results related to conjectures.
First we give in Section 5 results on the fourth conjecture since resolving this conjecture would be a basis for treating the others. Results on Conjectures 1, 2, and 3 are presented in Sections 6, 7 and 8 respectively. Section 9 is devoted to conclusions.

2 Some Definitions

Let \( G \) be a simple graph with \( n \) vertices. We write \( V(G) \) for the vertex set of \( G \), and \( E(G) \) for the edge set of \( G \).

The characteristic polynomial \( \det(xI - A) \) of a \((0,1)\)-adjacency matrix \( A \) of \( G \) is called the characteristic polynomial of \( G \) and denoted by \( p_G(x) \). The eigenvalues of \( A \) (i.e., the zeros of \( \det(xI - A) \)) and the spectrum of \( A \) (which consists of the \( n \) eigenvalues) are also called the eigenvalues and the spectrum of \( G \), respectively. The eigenvalues of \( G \) are usually denoted by \( \lambda_1, \lambda_2, \ldots, \lambda_n \); they are real because \( A \) is symmetric. Unless we indicate otherwise, we shall assume that \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) and use the notation \( \lambda_i = \lambda_i(G) \) for \( i = 1, 2, \ldots, n \).

The eigenvalues of \( A \) are the numbers \( \lambda \) satisfying \( Ax = \lambda x \) for some non-zero vector \( x \in \mathbb{R}^n \). Each such vector \( x \) is called an eigenvector of the matrix \( A \) (or of the labelled graph \( G \)) belonging to the eigenvalue \( \lambda \).

Let \( G \) be a graph with \( n \) vertices and \( m \) edges. Let \( \lambda_1(G) = \lambda_1, \lambda_n(G) = \lambda_n \) be the largest and the least eigenvalue of \( G \) respectively. Let \( \lambda_1(G) = X_1 \). The largest eigenvalue is also called the index or the spectral radius of the graph. If \( G \) is connected, there is a positive eigenvector belonging to \( \lambda_1 \). The unique positive unit eigenvector of \( \lambda_1 \) is the principal eigenvector of \( G \).

The difference between the index and the average vertex degree is called the irregularity of a graph (Collatz and Sinogowitz 1957).

The quantity \( \lambda_1 - \lambda_n \) is called the spectral spread of the graph.

As usual, \( K_n, C_n \) and \( P_n \) denote respectively the complete graph, the cycle and the path on \( n \) vertices. Further, \( K_{m,n} \) denotes the complete bipartite graph on \( m + n \) vertices.

The union of (disjoint) graphs \( G \) and \( H \) is denoted by \( G \cup H \), while \( mG \) denotes the union of \( m \) disjoint copies of \( G \).

We shall continue by giving definitions of some specific notions.

A complete split graph with parameters \( n, q (q \leq n) \), denoted by \( CS(n, q) \), is a graph on \( n \) vertices consisting of a clique on \( q \) vertices and a stable set on the remaining \( n - q \) vertices in which each vertex of the clique is adjacent to each vertex of the stable set.

A fanned complete split graph with parameters \( n, q, t(n \geq q \geq t) \), denoted by \( FCS(n, q, t) \), is a graph (on \( n \) vertices) obtained from a complete split graph \( CS(n, q) \) by connecting a vertex from the stable set by edges to \( t \) other vertices of the stable set.

A nested split graph with parameters \( n, q, k; p_1, p_2, \ldots, p_k; q_1, q_2, \ldots, q_k \), denoted by \( NS(n, q, k; p_1, p_2, \ldots, p_k; q_1, q_2, \ldots, q_k) \), is a graph on \( n \) vertices consisting of a clique on \( q \) vertices and \( k \) stable sets \( S_1, S_2, \ldots, S_k \) of cardinalities
\( p_1, p_2, \ldots, p_k \) vertices respectively; vertices in these stable sets have \( q_1, q_2, \ldots, q_k \) neighbors in the clique respectively, the set of neighbors of \( S_i+1 \) being a proper subset of the set of neighbors of \( S_i \) for \( i = 1, 2, \ldots, k-1 \). The nested split graphs have a stepwise adjacency matrix (Cvetković et al. 1997, pp. 60–74).

A pineapple with parameters \( n, q (q \leq n) \), denoted by \( PA(n, q) \), is a graph on \( n \) vertices consisting of a clique on \( q \) vertices and a stable set on the remaining \( n-q \) vertices in which each vertex of the stable set is adjacent to a unique vertex of the clique.

A fanned pineapple of type \( i (i=1, 2) \) with parameters \( n, q, t (n \geq q \geq t) \), denoted by \( FPA_i(n, q, t) \), is a graph (on \( n \) vertices) obtained from a pineapple \( PA(n, q) \) by connecting a vertex from the stable set by edges to \( t \) vertices of the clique when \( i=1 \) (\( 0 \leq t \leq q-2 \)), and to \( t \) vertices of the stable set when \( i=2 \) (\( 0 \leq t < n-q \)).

We have \( FPA_i(n, q, 0) = PA(n, q) \) for \( i=1, 2 \).

3 AGX Conjectures on the Index of a Graph

The following conjectures related to the index of a graph have been formulated after some experiments with the system AutoGraphiX (AGX).

**Conjecture 1.** The most irregular connected graph on \( n \) vertices \((n \geq 10)\) vertices is a pineapple \( PA(n, q) \) in which the clique size \( q \) is equal to \( \lceil \frac{n}{2} \rceil + 1 \).

This assertion has been established by AGX for \( n = 10, 11, \ldots, 17 \). For smaller values of \( n \) the maximal graph is again a pineapple (reduced to a star for \( n = 5, 6, 7 \)).

**Conjecture 2.** Given \( n \), the maximal value of the spectral spread of a graph on \( n \) vertices is obtained for a complete split graph \( CS(n, q) \) with an independent set of size \( n-q = \lceil \frac{n}{3} \rceil \).

**Conjecture 3.** The maximal graphs on \( n \) vertices for the function \( \lambda_1 + \lambda_\bar{1} \) are the complete split graphs \( CS(n, q) \) with the clique size equal or close to \( \frac{n}{3} \).

More precisely, for any simple graph \( G \), with complement \( \bar{G} \), spectral radius \( \lambda_1(G) \) and \( n \) vertices we have

\[
\lambda_1(G) + \lambda_1(\bar{G}) \leq \frac{4}{3}n - \frac{5}{3} + \left\{ \begin{array}{ll}
f_1(n) & \text{if } n \equiv 1 \pmod{3} \vspace{1mm} \\
0 & \text{if } n \equiv 2 \pmod{3} \vspace{1mm} \\
f_2(n) & \text{if } n \equiv 0 \pmod{3} \end{array} \right.
\]

where \( f_1(n) = \frac{3n-2-\sqrt{9n^2-12n+12}}{6} \) and \( f_2(n) = \frac{3n-1-\sqrt{9n^2-6n+9}}{6} \).

This bound is sharp and attained if and only if \( G \) or \( \bar{G} \) is a complete split graph with an independent set on \( \lfloor \frac{n}{2} \rfloor \) vertices (and also on \( \lceil \frac{n}{3} \rceil \) vertices if \( n \equiv 2 \pmod{3} \)).

We shall describe in some detail the use of AGX in formulating Conjecture 3.
Additional experiments have shown that maximal graphs for $\lambda_1 + \overline{\lambda}_1$ for given $n$ and $m$ are complete split graphs or fanned complete split graphs with a few exceptions.

When looking for extremal graphs with the system AutoGraphiX (AGX), using the variable neighborhood search metaheuristic, we defined the objective function as $\lambda_1(G) + \lambda_1(\overline{G})$ to be maximized over the class of all graphs of order from 4 to 24. To be coherent in our investigations, we required the graph $G$, but not necessarily its complement $\overline{G}$, to be connected. This constraint is without loss of generality because of the fact that at least one of the complementary graphs $G$ and $\overline{G}$ is connected.

For a fixed order $n$, the extremal graph $G$ is composed of a clique on $q$ vertices and a stable set with $s$ vertices in which every vertex is connected to all vertices of the clique. When we observed the values of $q$ and $s$ for different graphs, we found the following:

$$q = \begin{cases} \lfloor \frac{n}{3} \rfloor & \text{if } n \equiv 1 \pmod{3} \\ \frac{n}{3} & \text{if } n \equiv 0 \pmod{3} \end{cases}$$ and $$s = \begin{cases} \lceil \frac{2n}{3} \rceil & \text{if } n \equiv 1 \pmod{3} \\ \frac{2n}{3} & \text{if } n \equiv 0 \pmod{3} \end{cases}$$

While the experiments show uniformity for the cases $n \equiv 0 \pmod{3}$ and $n \equiv 1 \pmod{3}$, it was not the case when $n \equiv 2 \pmod{3}$. Sometimes we have $q = \lfloor \frac{n}{3} \rfloor$ and $s = \lceil \frac{2n}{3} \rceil$ and other times, we have $q = \lfloor \frac{n}{3} \rfloor$ and $s = \lfloor \frac{2n}{3} \rfloor$. We decided to examine the two cases interactively on AGX for every $n$, and we observed that the objective function has the same value in both cases ($q = \lfloor \frac{n}{3} \rfloor$ or $q = \lceil \frac{n}{3} \rceil$).

AGX did not find any conjecture on the relation between the objective function $\lambda_1(G) + \lambda_1(\overline{G})$ and the order when using all the presumably extremal graphs obtained by AGX. But when we separated the set of graphs into three subsets, with $n \equiv 0 \pmod{3}$ for the first subset, $n \equiv 1 \pmod{3}$ for the second one and $n \equiv 2 \pmod{3}$ for the third one, AGX did not find anything about the two first subsets but suggested the following linear relation for the third one ($n \equiv 2 \pmod{3}$)

$$\lambda_1(G) + \lambda_1(\overline{G}) = \frac{4}{3}n - \frac{5}{3}$$

Conjecture 3 suggests a result of Nordhaus-Gaddum type. Such results have a long history.

Nordhaus and Gaddum (1956) proved that

$$2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n + 1$$

and

$$n \leq \chi(G) \cdot \chi(\overline{G}) \leq \frac{(n + 1)^2}{4}.$$
a graph invariant, *i.e.*, a function defined for all graphs and whose value is independent of vertex or edge labelling. Classical Nordhaus-Gaddum relations are of the following form:

\[ l_1(n) \leq i(G) + i(\bar{G}) \leq u_1(n) \]

and

\[ l_2(n) \leq i(G) \cdot i(\bar{G}) \leq u_2(n). \]

In more general form, the lower and upper bounding functions may depend on several variables.

Nosal (1970) and Amin and Hakimi (1972) independently proved that

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

The lower bound is attained if and only if the graph is regular.

It is proved in (Nikiforov 2002) that

\[ \lambda_1(G) + \lambda_1(\bar{G}) \leq \sqrt{(2 - 1/k - 1/\bar{k})n(n - 1)}. \]

where \( k \) and \( \bar{k} \) are the size of a maximal clique in \( G \) and \( \bar{G} \) respectively.

The difficulty in proving Conjectures 2 and 3 is that we have almost no lemmas on the behavior of the corresponding invariant under local graph transformations (which we do have with the largest eigenvalue, involved in Conjecture 4 below). Experiments with GRAPH, newGRAPH and AGX would be useful in producing conjectures for such lemmas (e.g. adding an edge, rotating an edge etc.). However, for the irregularity of a graph (involved in Conjecture 1) we do have such lemmas (see Section 6).

The common characteristic of the three conjectures is that the graph invariant involved is the sum or the difference of two invariants which behave differently when varying some parameters (e.g. the number of edges).

4 Maximal Index of Connected Graphs with Given Numbers of Vertices and Edges

The three conjectures are related to the problem of finding the maximal index of connected graphs with given \( m \) and \( n \). This problem has been studied for some time. See (Cvetković et al. 1997) for a survey of results and for the decades long history of this problem.

Experiments with AGX gave as a maximal graph a pineapple or a fanned pineapple of the first kind for \( n = 10 \) and all \( m \). A graph depicting the dependency of \( \lambda_1 \) on \( m \) has been produced. The graph roughly represents a straight line but really consists of several concave segments corresponding to families of fanned pineapples with a fixed clique. However, having in mind results of
Bruzual and Solheid (1986) and Cvetković and Rowlinson (1988) (see (Snellman 2003) for corresponding results for digraphs) other graphs could appear as maximal graphs with higher values of $n$.

However, the following partial results and a conjecture have been obtained independently of the system AGX.

Let $H(n, n + k)$ be the set of all connected graphs with $n$ vertices and $n + k$ edges, and let $G_{n,k}$ and $H_{n,k}$ be the graphs defined in (Cvetković and Rowlinson 1988). These graphs are fanned pineapple graphs of types 1 and 2 respectively: using the notation of Section 2 we have $G_{n,k} = FPA_1(n, d, t)$ and $H_{n,k} = FPA_2(n, 1, k + 1)$.

We can write $k$ in the form $k = (d^{-1}) + t - 1$, where $0 \leq t \leq d - 2$, and we suppose that $k \geq 3$. Denote the index of a graph $G$ by $\rho(G)$. We start by comparing $\rho(G_{n,k})$ with $\rho(H_{n,k})$.

**Lemma 1.** Let $k = (d^{-1}) + t - 1$, and suppose that $3 \leq k < n - 3$. If $\rho(G_{n,k}) = \rho(H_{n,k}) = \rho$, then $\rho$ is a root (in fact, the largest root) of the cubic equation $c_k(x) = 0$, where

$$c_k(x) = px^3 + qx^2 + rx + s,$$

with

$$p = (d - 2)(d - 3)(d - 1)(d - 4) + 4t,$$
$$q = -(d - 1)(d - 2)(d - 3)(d^2 - 5d + 8) - 4(d^3 - 8d^2 + 19d - 15)t - 4(2d - 3)t^2,$$
$$r = -(d - 1)(d - 2)^3(d - 3) - (d - 2)(d^3 - 4d^2 - 3d + 10)t - 2d(3d - 2)t^2 - 8t^3,$$
$$s = t(d - 2 - t)[(d - 1)(d - 2) + 2t][(d - 1)(d - 4) + 2t].$$

**Proof.** If $k = 3$, then $d = 4$, $t = 1$; if $k = 4$, then $d = 4$, $t = 2$; while for $k \geq 5$ we have $d \geq 4$, $t \geq 1$. Suppose first that $d \geq 5$, $t = 0$. In this case, it may be verified that the equation $c_k(x) = 0$ has roots $x = -1$, $x = 0$, $x = d + \frac{4}{d - 1}$. The result then follows from (Bell 1991, Lemma 1). We can now assume that $d \geq 4$, $t \geq 1$.

Let $G_{n,k}$ have index $\gamma$, principal eigenvector $y$, and stepwise adjacency matrix $B$. Then $y_2 = \ldots = y_{t+1}$, $y_{t+2} = \ldots = y_d$, and $y_{d+2} = \ldots = y_n$. Similarly, let $H_{n,k}$ have index $\chi$, principal eigenvector $z$, and stepwise adjacency matrix $C$. We have $z_2 = \ldots = z_{k+3}$, and $z_{k+4} = \ldots = z_n$. Then $y^T(B - C)z = (\chi - \gamma)y^Tz$, and it may be verified that we also have $y^T(B - C)z = r(Qz_3 - y_{n+2})$, where $r = (d^{-2}) + t - 1$, and $rQ = \frac{1}{2}(d - 3)(2t - d)y_2 + (d - 3)(d - t - 1)y_d + (t - 1)y_{d+1}$. By solving the eigenvalue equations for $y_2, y_d, y_{d+1}$ and $y_n$, we obtain

$$Q = \frac{(d^2 - 5d + 2t + 4)\gamma^2 + 2(t - 1)\gamma^2 + (d - t - 2)(d - 3)(2t - d) - 2(t - 1)\gamma}{(d^2 - 5d + 2t + 4)\gamma^2 - (d - t - 2)\gamma - (d - t - 2)\gamma + t(2t - d)}.$$

Similarly,

$$\frac{z_2}{z_3} = \frac{\chi + \frac{1}{2}(d^2 - 3d + 2) + t}{\chi + 1}.$$
If $\gamma = \chi = \rho$, then $\frac{\gamma}{\gamma_n} = \frac{\chi}{\chi_n}$, and it may be verified that this implies that $\rho$ satisfies the equation $c_k(x) = 0$. Also, it is not difficult to show that $\rho$ is the largest root of this equation.

We will denote the largest root of $c_k(x)$ by $\rho_k$, in order to show its dependence on $k$.

**Lemma 2.** Let $k = \left(\frac{d-1}{2}\right) + t - 1$, and suppose that $3 \leq k < n - 3$. Then one of the following holds:

(i) $\rho(H_{n,k}) < \rho(G_{n,k}) < \rho_k$;
(ii) $\rho(H_{n,k}) = \rho(G_{n,k}) = \rho_k$;
(iii) $\rho(H_{n,k}) > \rho(G_{n,k}) > \rho_k$;

**Proof.** Here (ii) is the situation of Lemma 1. For (i), suppose that $\chi < \gamma$ (where, as before, $\gamma$ and $\chi$ denote $\rho(G_{n,k})$ and $\rho(H_{n,k})$, respectively). Then $y^T(B - C)z > 0$, and therefore $\frac{\gamma}{\gamma_n} > \frac{\chi}{\chi_n}$. This implies that $c_k(\gamma) < 0$, so that $\gamma < \rho_k$. The proof of (iii) is similar.

We find experimentally that, for a fixed value of $k$, $\rho(H_{n,k})$ is less than $\rho(G_{n,k})$ for small $n$, but greater than $\rho(G_{n,k})$ for large $n$. There is a precise value of $n$ (depending on $k$) at which the two are equal, and we can find this as follows. From equation (14) of (Bell 1991), $\chi$ is the largest root of $h(x)$, where

$$h(x) = x^4 - (n + k)x^2 - 2(k + 1)x + (k + 1)(n - k - 3).$$

Thus $h(x) = 0$ if and only if

$$n = x^2 + 1 - \frac{(k + 1)(2x + k + 2)}{x^2 - k - 1}.$$

We therefore define a function $f(k)$ by

$$f(k) = \rho_k^2 + 1 - \frac{(k + 1)(2\rho_k + k + 2)}{\rho_k^2 - k - 1}.$$

It can be proved that $\rho_k > d$, and therefore $\rho_k^2 > k + 1$, so that $f$ is well-defined. It is also easily proved that $f(k) > k + 3$, which ensures that $H_{n,k}$ is defined whenever $n \geq f(k)$. From Lemma 2, we deduce:

**Lemma 3.** Let $k = \left(\frac{d-1}{2}\right) + t - 1$, and suppose that $3 \leq k < n - 3$. Then we have:

(i) $\rho(H_{n,k}) < \rho(G_{n,k}) < \rho_k$ if $n < f(k)$;
(ii) $\rho(H_{n,k}) = \rho(G_{n,k}) = \rho_k$ if $n = f(k)$;
(iii) $\rho(H_{n,k}) > \rho(G_{n,k}) > \rho_k$ if $n > f(k)$.

Of course, if $f(k)$ is not an integer, then $\rho(H_{n,k}) = \rho(G_{n,k})$ cannot occur. Lemma 3 suggests the following conjecture:
Conjecture 4. Let $k \geq 3$, and let $G$ be a graph of maximal index in $\mathcal{H}(n,n+k)$.

(i) If $n < f(k)$ then $G = G_{n,k}$.
(ii) If $n = f(k)$ then $G = G_{n,k}$ or $H_{n,k}$.
(iii) If $n > f(k)$ then $G = H_{n,k}$.

The following table of the values of $c_k(x), \rho_k$ and $f(k)$ for small values of $k$ is obtained by direct calculation:

<table>
<thead>
<tr>
<th>$k$</th>
<th>$c_k(x)$</th>
<th>$\rho_k$</th>
<th>$f(k)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$8x^3 - 32x^2 - 48x + 16$</td>
<td>5.10</td>
<td>24.24</td>
</tr>
<tr>
<td>4</td>
<td>$16x^3 - 80x^2 - 160x$</td>
<td>6.53</td>
<td>41.12</td>
</tr>
<tr>
<td>5</td>
<td>$24x^3 - 192x^2 - 216x$</td>
<td>9</td>
<td>80</td>
</tr>
<tr>
<td>6</td>
<td>$48x^3 - 240x^2 - 336x + 168$</td>
<td>6.06</td>
<td>32.98</td>
</tr>
<tr>
<td>7</td>
<td>$72x^3 - 344x^2 - 608x + 256$</td>
<td>6.07</td>
<td>32.01</td>
</tr>
<tr>
<td>8</td>
<td>$96x^3 - 504x^2 - 1080x$</td>
<td>6.88</td>
<td>42.82</td>
</tr>
<tr>
<td>9</td>
<td>$120x^3 - 840x^2 - 960x$</td>
<td>8</td>
<td>60</td>
</tr>
</tbody>
</table>

For a given $n$, the maximal graph is $H_{n,k}$ for $k$ sufficiently small. The “dual” conjecture that there is a function $g(n)$ such that for a given $n$ the maximal graph is $H_{n,k}$ if $k < g(n)$ and $G_{n,k}$ if $k > g(n)$ is unlikely to be true, as the following graph of the function $f(k)$ shows.

Looking at the graph, we see that for fixed $n$ between 50 and 60 the character of the maximal graph changes several times as $k$ increases. This observation highlights the difficulty of the problem of finding a graph with maximal index among the graphs with fixed numbers of vertices and edges.
5 Results related to Conjecture 4

We shall first treat Conjecture 4 since the results are helpful in treating the other conjectures.

Conjecture 4 has been proved for all \( k \) of the form \( k = \binom{m}{2} - 1 \) \((m \geq 4)\): see (Bell 1991). (Note that this includes the case \( k = 5 \).) It is also true when \( k = 3, 4, 6 \). This is immediate when \( k = 3 \), because \( G_{n,3} \) and \( H_{n,3} \) are the only graphs with stepwise adjacency matrices in this case.

Proof when \( k = 4 \). In addition to \( G_{n,4} \) and \( H_{n,4} \), there is just one graph \( G \) with a stepwise adjacency matrix. This has adjacency matrix \( A = (a_{ij}) \), where 

\[
a_{1j} = 1 \quad (2 \leq j \leq n), \quad a_{2j} = 1 \quad (j = 3, 4, 5, 6), \quad a_{34} = 1, \quad \text{and all other } a_{ij} \text{ with } i < j \text{ are equal to } 0.
\]

Let \( G \) have index \( \rho \), with principal eigenvector \( x \).

Suppose first that \( n > f(4) \). Then, by Lemma 3, \( \chi > \gamma \), and we have to prove that \( \rho < \chi \). We therefore suppose, by way of contradiction, that \( \rho \geq \chi \). We have 

\[
\frac{z_2}{z_3} \leq \frac{q}{x_n}.
\]

Using the eigenvalue equations, we obtain that

\[
\frac{q}{x_n} = \frac{2x_3 - x_2}{x_n} < \frac{x_3}{x_2} = \frac{\rho^3 + \rho^2}{\rho^3 - \rho^2 - 4\rho + 2} < \frac{\rho^2 + \rho}{\rho^2 - \rho - 4}.
\]

We also have 

\[
(\chi - \gamma)y^Tz = 2(y_n z_2 - Q z_3), \quad \text{where } Q = y_4.
\]

Thus 

\[
\frac{z_2}{z_3} > \frac{Q}{y_n} = \frac{\gamma^2 + \gamma}{\gamma^2 - \gamma - 4}.
\]

Now \( \frac{x_3 - x_2}{x_2} \) is a decreasing function for \( x > 0 \), and it follows that

\[
\frac{z_2}{z_3} > \frac{q}{x_n},
\]

a contradiction. Therefore \( H_{n,4} \) has largest index whenever \( n > f(4) \). A trivial modification proves the result when \( n = f(4) \), and similar arguments can be used for the case \( n < f(4) \).

In the case \( k = 6 \) there are three graphs to consider (instead of just one), but analogous arguments can be deployed to show that none of these has maximal index for any \( n \).

It was proved in (Cvetković and Rowlinson 1988) that the maximal graph is \( H_{n,k} \) for given \( k \) and sufficiently large \( n \).

Theoretically we know that maximal graphs have a stepwise adjacency matrix (Cvetković et al. 1997, pp. 60–74). Note that graphs with a stepwise adjacency matrix are exactly the nested split graphs. Moreover, S. Simić et al. (2004) have recently proved the following proposition. Alternatively, it follows immediately from the stepwise nature of an adjacency matrix.
**Proposition 1.** A graph is a nested split graph if and only if it does not contain as an induced subgraph any of the graphs $P_4, 2K_2, C_4$.

With this characterization one can instruct AGX to search for maximal graphs only among nested split graphs, and this would perhaps make it possible to find the extremal graphs for $n$ up to 60. Stepwise matrices can easily be enumerated by counting the number of zig-zag lines between two fixed points in a square grid.

Since the set of forbidden subgraphs in Proposition 1, namely $P_4, 2K_2, C_4$, is closed under the operation of complementation the following proposition is straightforward. Alternatively, it follows immediately from the stepwise nature of an adjacency matrix.

**Proposition 2.** The complement of a nested split graph is also a nested split graph.

### 6 Results related to Conjecture 1

We start with a new proof of an old relevant result.

Let $G$ be a simple graph with $n$ vertices, $m$ edges, index $\lambda_1$ and average vertex degree $\bar{d}$. In (Hong 1988) it is proved that $\lambda_1 \leq \sqrt{2m - n + 1}$, with equality if and only if $G$ is a complete graph $K_n$ or a star $K_{1,n-1}$. Using an inequality between arithmetic and geometric means, we get

\[
\lambda_1 \leq \sqrt{2m - n + 1} = 2\sqrt{\frac{2m - n + 1}{4}} = 2\sqrt{\frac{n}{4} - \frac{2m - n + 1}{n}}.
\]

Since the average vertex degree is given by $\bar{d} = \frac{2m}{n}$, we actually get for the irregularity

\[
\lambda_1 - \bar{d} \leq \frac{n}{4} - 1 + \frac{1}{n}.
\]

This upper bound on irregularity is part of Proposition 7 of (Bell 1992) deduced there from Hong’s bound (Hong 1988) in a different way.

The bound is indeed very close to what we need to prove. Namely, $\frac{n}{4} - 1$ is the best-fitting linear function for irregularity of pineapples in which the clique size is equal to $\lceil \frac{n}{2} \rceil + 1$: its index is slightly larger than $\lceil \frac{n}{2} \rceil$ (the index is a root of a cubic equation and a nice closed-form formula is impossible) and its average degree is approximately $\frac{n}{4} + \frac{1}{2} - \frac{2}{n}$.

In treating Conjecture 1 the perturbation theory for graph eigenvalues (Chapter 6 of (Cvetkovic et al. 1997)) could be useful. We know from Section 5 that a connected graph of maximal irregularity is a nested split graph.

**Lemma 4.** If the connected graph $G$ has principal eigenvector $(x_1, \ldots, x_n)^T$ with non-adjacent vertices $i,j$ such that $x_i x_j \geq 1/n$, then the irregularity of $G + ij$...
exceeds that of \( G \). If \( i, j \) are non-adjacent vertices such that \( x_i x_j \leq 1/n \), then the irregularity of \( G - ij \) exceeds that of \( G \).

The proof is carried out by a Rayleigh type argument (Cvetković et al. 1997, p. 143).

On the basis of Lemma 4 the following property of maximal irregular graphs can be established. The property is sufficient but not necessary for a graph to be a nested split graph.

**Proposition 3.** Let \( G \) be a maximal irregular connected graph with principal eigenvector \((x_1, \ldots, x_n)^T\). Then \( x_i x_j < 1/n \), whenever vertices \( i, j \) are non-adjacent and \( x_i x_j > 1/n \), whenever \( ij \) is a non-pendant edge.

In addition, all lemmas describing the behavior of the largest eigenvalue under transformations that do not change the number of edges are relevant also to the irregularity.

The following derivations might be useful in relations with Lemma 1.

For a normalized eigenvector \( x \) of an eigenvalue \( \lambda \) we have

\[
Ax = \lambda x, \quad x^T Ax = \lambda x, \quad x^T x = 1.
\]

Let \( j = (1, 1, \ldots, 1)^T \) and let \( \beta \) be the main angle of \( \lambda \). Then

\[
\left( \sum x_i \right)^2 = (j^T x)^2 = (\sqrt{n} \beta)^2 = n \beta^2
\]

\[
= \sum x_i^2 + 2 \sum x_i x_j = 1 + 2 \sum_{i < j, i \text{ adj } j} x_i x_j + 2 \sum_{i < j, i \text{ non-adj } j} x_i x_j
\]

\[
= 1 + x^T Ax + 2 \sum_{i < j, i \text{ non-adj } j} x_i x_j
\]

\[
= 1 + \lambda + 2 \sum_{i \text{ adj } j} x_i x_j.
\]

We have

\[
\sum_{i \text{ non-adj } j} x_i x_j = \frac{n \beta^2 - 1 - \lambda}{2}.
\]

For the average value \( E(x_i, x_j) \) of \( x_i x_j \) over all pairs of non-adjacent vertices \( i \) and \( j \) we obtain the following asymptotic inequality:

\[
E(x_i, x_j) \bigg|_{i \text{ non-adj } j} = \frac{n \beta^2 - 1 - \lambda}{2m} = \frac{n \beta^2 - 1 - \lambda}{2(n(n - 1)/2 - m)}
\]

\[
= \frac{n \beta^2 - 1 - \lambda}{n(n - 1) - 2m} = \frac{\beta^2 - 1/n - \lambda/n}{(n - 1) - 2m/n} \sim \frac{\beta^2}{(n - 1)}
\]
Hence, we have proved the following proposition.

**Proposition 4.** Let $\beta$ be the main angle of an eigenvalue $\lambda$ of a graph $G$. Let $E(x_i,x_j)$ be the average value of $x_i x_j$ over all pairs of non-adjacent vertices $i$ and $j$ of $G$. We have the following asymptotic inequality:

$$E(x_i,x_j)_{i \text{ non-adj} j} > \frac{\beta^2}{n}.$$  

This proposition can perhaps help in some situations to prove the existence of a pair of non-adjacent vertices to which Lemma 1 can be applied. By repeating such an argument one could force the addition of all possible edges, thus forming a clique.

### 7 Results related to Conjecture 2

Little can be found in the literature concerning the spectral spread of a graph. All graphs whose spectral spread does not exceed 4 are determined in (Petrović 1983). The spectral spread of unicyclic graphs has been studied in (Shu and Wu 2003).

However, Conjecture 2 did appear in the literature (Gregory et al. 2001) but remained unsolved. It is noted in (Gregory et al. 2001) that the conjecture has been verified by computer for graphs up to 9 vertices.

Let us consider the matrix associated to the divisor (Chapter 4 of Cvetković et al. 1995) of a complete split graph with $q$ vertices in the clique and $n-q$ in the stable set,

$$A = \begin{bmatrix} q-1 & n-q \\ q & 0 \end{bmatrix}.$$  

The index of the graph is exactly the largest eigenvalue of $A$, which is

$$\lambda_1 = \frac{q-1}{2} + \sqrt{4qn - 3q^2 - 2q + 1}.$$  

### 8 Results related to Conjecture 3

In (Hong et al. 2001), Y. Hong, J. L. Shu and K. Fang proved that for a simple connected graph $G$ with order $n$, size $m$, minimum degree $\delta$ and spectral radius $\lambda_1(G)$:

$$\lambda_1(G) \leq \frac{\delta - 1 + \sqrt{(\delta + 1)^2 + 4(2m - \delta n)}}{2} \quad (1)$$
and equality holds if and only if $G$ is either a regular graph or a graph in which each vertex is of degree either $\delta$ or $n-1$.

Further, R. P. Stanley (1987) showed that the spectral radius of any graph with $m$ edges satisfies:

$$\lambda_1(G) \leq \frac{-1 + \sqrt{1 + 8m}}{2}$$  \hspace{1cm} (2)

and equality occurs if and only if there exists $k$ such that $m = k(k-1)/2$ and $G$ is the disjoint union of the complete graph $K_k$ and $n-k$ isolated vertices.

When examining the extremal graphs given by AGX in relation to the above two results, we can see that they are among the graphs for which the first upper bound is sharp, and the complements are among those for which the second one is sharp. From this remark, it seems to be of interest to study the two bounds together.

Let us consider a complete split graph $G$ on $n$ vertices. The inequality (1) is sharp for $G$ and (2) is sharp for $\bar{G}$. For such a graph we have

$$m = \delta(n - \delta) + \delta(\delta - 1)/2 = \frac{(2n-1)\delta - \delta^2}{2}$$  \hspace{1cm} (3)

and so we obtain the following inequalities

$$\lambda_1(G) + \lambda_1(\bar{G}) \leq \frac{(\delta - 1 + \sqrt{(\delta + 1)^2 + 4(2m - \delta n)}) + (-1 + \sqrt{1 + 8(n(n-1)/2 - m)}}{2}$$

$$\lambda_1(G) + \lambda_1(\bar{G}) \leq \frac{2n - 3 - \delta + \sqrt{1 + 2(2n - 1)\delta - 3\delta^2}}{2}.$$  

Let us consider the function

$$f(x) = \frac{2n - 3 - x + \sqrt{1 + 2(2n - 1)x - 3x^2}}{2}.$$  

To obtain an upper bound for the objective function it is sufficient to find the maximal value of this function. The derivative of this function is

$$f'(x) = -\frac{1}{2} + \frac{2n - 1 - 3x}{\sqrt{1 + 2(2n - 1)x - 3x^2}}$$

which is zero if and only if

$$2n - 1 - 3x = \sqrt{1 + 2(2n - 1)x - 3x^2}$$

that is for $x = x^* = \frac{2n - \sqrt{n^2 - n + 1}}{3}$.  

It is easy to see that $f'(x) < 0$ for $x^* < x \leq n - 1$ and $f'(x) > 0$ for $1 \leq x < x^*$. Then we conclude that the function $f$ is increasing for
1 \leq x \leq x^*, \text{ decreasing for } x^* \leq x \leq n - 1 \text{ and its maximum value is obtained for } x = x^* = \frac{2n-\sqrt{n^2-n+1}}{3}.

This is if we consider \( x \) as a continuous variable, but when considering it as an integer variable the maximum value of the function is attained for \( x_1 = \lfloor x^* \rfloor \) or for \( x_2 = \lceil x^* \rceil \) (\( x^* \) can never be an integer if \( n > 0 \)).

By easy algebraic computation, we can show that

\[
\frac{n-1}{3} < x^* < \frac{n}{3} \quad \text{if } n \equiv 0 \pmod{3},
\]
\[
\frac{n}{3} < x^* < \frac{n+1}{3} \quad \text{if } n \equiv 1 \pmod{3},
\]
\[
\frac{n+1}{3} < x^* < \frac{n+2}{3} \quad \text{if } n \equiv 2 \pmod{3}.
\]

From this, we can compute \( \lfloor x^* \rfloor \) and \( \lceil x^* \rceil \) and get:

\[
\lfloor x^* \rfloor = \begin{cases} 
\frac{n-1}{3} & \text{if } n \equiv 0 \pmod{3} \\
\frac{n+1}{3} & \text{if } n \equiv 1 \pmod{3} \\
\frac{n+2}{3} & \text{if } n \equiv 2 \pmod{3}
\end{cases}
\]
\[
\lceil x^* \rceil = \begin{cases} 
\frac{n-1}{3} & \text{if } n \equiv 0 \pmod{3} \\
\frac{n}{3} & \text{if } n \equiv 1 \pmod{3} \\
\frac{n+1}{3} & \text{if } n \equiv 2 \pmod{3}
\end{cases}
\]

Now, to know the maximum value of the function, we have to compute and compare \( f(\lfloor x^* \rfloor) \) and \( f(\lceil x^* \rceil) \) in each case.

1. Case \( n \equiv 0 \pmod{3} \)
   In this case, it is easy to see that:

   \[
f\left(\frac{n}{3}\right) = \frac{5n + \sqrt{9n^2 - 6n + 9}}{6} \geq f\left(\frac{n-1}{3}\right) = \frac{5n + \sqrt{9n(3n-8)}}{6} - 1
\]

   So the maximum is attained for \( x = \lfloor x^* \rfloor \) and its value is

   \[
f\left(\frac{n}{3}\right) = \frac{5n + \sqrt{9n^2 - 6n + 9}}{6} - \frac{3}{2} = \frac{4n-5}{3} - \frac{3n-1-\sqrt{9n^2-6n+9}}{6}
\]

2. Case \( n \equiv 1 \pmod{3} \)
   In this case, it is easy to see that:

   \[
f\left(\frac{n-1}{3}\right) = \frac{5n + \sqrt{9n^2 - 12n + 12}}{6} - \frac{4}{3} \geq f\left(\frac{n+2}{3}\right) = \frac{5n + \sqrt{9n^2 + 6n - 15 - 11}}{6}
\]

   So the maximum is attained for \( x = \lceil x^* \rceil \) and its value is

   \[
f\left(\frac{n-1}{3}\right) = \frac{5n + \sqrt{9n^2 - 12n + 12}}{6} - \frac{4}{3} = \frac{4n-5}{3} + \frac{3n-2-\sqrt{9n^2-12n+12}}{6}
\]

3. Case \( n \equiv 2 \pmod{3} \)
   In this case, we have two maxima:

   \[
f\left(\frac{n-2}{3}\right) = f\left(\frac{n+1}{3}\right) = \frac{4}{3} n - \frac{5}{3}.
\]
Hence, we have proved Conjecture 3 in the special case of complete split graphs (since relation (3) was used).

We can prove Conjecture 3 for a broad class of graphs very easily. Let $\delta, \Delta$ be the minimal and maximal vertex degree of a graph $G$ respectively and $\bar{\delta}, \bar{\Delta}$ the corresponding quantities for $\bar{G}$.

**Proposition 5.** If $\Delta - \delta \leq \frac{2n-2}{3}$, then

$$\lambda_1(G) + \lambda_1(\bar{G}) \leq \frac{4}{3} n - \frac{5}{3}$$

**Proof.** Since $\lambda_1(G) \leq \Delta$, $\lambda_1(\bar{G}) \leq \bar{\Delta}$ and $\bar{\Delta} = n - 1 - \delta$, the conclusion follows.

### 9 Conclusion

Conjecture 3 was formulated by P. Hansen and his doctoral student M. Aouchiche in early 2004. During his visit to Institute GERAD, Montreal, in May 2004, D. Cvetković became acquainted with the conjecture and suggested experiments with AGX which have led to Conjectures 1 and 2. Experiments with AGX related to Conjecture 4 were not sufficient to make a reasonable conjecture since the existing theoretical results were indicating that the essential behaviour of the largest eigenvalue could be visible only on a higher number of vertices, thus beyond the capabilities of AGX. Therefore Conjecture 4 was formulated on a theoretical basis when the seven authors later agreed to work on the subject.

After one year and half the authors concluded that they cannot resolve any of the conjectures. Such an outcome was expected to some extent since from the beginning it was clear that the problems are very hard.

We shall summarize the main facts supporting the claim that the research problems related to Conjectures 1, 2, 3 and 4 are very complex.

1. **Complex behaviour of the maximal value of the index.** The results of comparing indices of the graphs $G_{n,k}$ and $H_{n,k}$, described in Section 4, indicate a strange and complicated behaviour of the maximal value of index. Several switches between these two graphs in this comparison with fixed $n$ and increasing $k$ (up to 10 changes for some values of $n$) reduce the expectation that the problem will be solved by existing spectral techniques. Since the index is involved in all conjectures, this pessimism extends also to Conjectures 1, 2 and 3. Also we repeat our remark from the end of Section 3 to the effect that the objective functions in Conjectures 1, 2 and 3 are composed of two graph invariants with mutually incoherent behaviour.

2. **Problems related to our conjectures have long been the subject of research without being solved.** The notion of irregularity was introduced in 1957 in the first mathematical paper on graph spectra (Collatz and Sinogowitz 1957), and a false conjecture concerning its upper bound was formulated. Conjecture 2 appeared in 2001 in (Gregory et al. 2001). Nordhaus-Gaddum type results
have a long tradition and in particular there were some efforts to find good upper bounds for \( \lambda_1(G) + \lambda_1(\bar{G}) \) as cited in Section 3. For more details on the maximum index problem see the book (Cvetković et al. 1997) and the expository article (Cvetković and Rowlinson 1990).

References


Aouchiche M.
École Polytechnique de Montréal,
2500, chemin de Polytechnique
Montréal, H3T 1J4 CANADA
e-mail: mustapha.aouchiche@gerad.ca

Bell F.K., Rowlinson P.
Mathematics and Statistics Group
Department of Computing Science and Mathematics
University of Stirling
FK9 4LA Stirling, Scotland, UK
e-mail: f.k.bell@maths.stir.ac.uk
e-mail: p.rowlinson@maths.stir.ac.uk

Cvetković D., Simić S.
Faculty of Electrical Engineering,
University of Belgrade,
P.O.Box 35–54,
11120 Belgrade,
Serbia and Montenegro
e-mail: ecvetkod@etf.bg.ac.yu
e-mail: ssimic@raf.edu.yu

Hansen P.
GERAD and École des Hautes Études Commerciales
3000 chemin de la Côte-Sainte-Catherine,
Montréal H3T 2A7, Canada
email: mustapha.aouchiche@gerad.ca
e-mail: pierre.hansen@gerad.ca

Stevanović D.
Faculty of Sciences,
University of Niš,
Višegradska 33,
18000 Niš,
Serbia and Montenegro
e-mail: dragance106@yahoo.com