Chapter 1

VARIABLE NEIGHBORHOOD SEARCH FOR EXTREMAL GRAPHS. XI. BOUNDS ON ALGEBRAIC CONNECTIVITY

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Abstract The algebraic connectivity $a(G)$ of a graph $G = (V, E)$ is the second smallest eigenvalue of its Laplacian matrix. Using the AutoGraphiX (AGX) system, extremal graphs for algebraic connectivity of G in function of its order $n = |V|$ and size $m = |E|$ are studied. Several conjectures on the structure of those graphs, and implied bounds on the algebraic connectivity, are obtained. Some of them are proved, e.g., if $G \neq K_n$

$$a(G) \leq \lfloor -1 + \sqrt{1 + 2m} \rfloor$$

which is sharp for all $m \geq 2$.

1. Introduction

Computers are increasingly used in graph theory. Determining the numerical value of graph invariants has been done extensively since the fifties of last century. Many further tasks have since been explored. Specialized programs helped, often through enumeration of specific families of graphs or subgraphs, to prove important theorems. The prominent example is, of course, the Four-color Theorem (Appel and Haken, 1977a,b, 1989; Robertson et al., 1997). General programs for graph enumeration, susceptible to take into account a variety of constraints and exploit symmetry, were also developped (see, e.g., McKay, 1990, 1998). An interactive approach to graph generation, display, modification and study through many parameters has been pioneered in the system Graph of Cvetković and Kraus (1983), Cvetković et al. (1981), and Cvetković and

Simić (1994) which led to numerous research papers. Several systems for obtaining conjectures in an automated or computer-assisted way have been proposed (see, e.g., Hansen, 2002, for a recent survey). The AutoGraphix (AGX) system, developed at GERAD, Montréal since 1997 (see, e.g., Caporossi and Hansen, 2000, 2004) is designed to address the following tasks: (a) Find a graph satisfying given constraints; (b) Find optimal or near-optimal values for a graph invariant subject to constraints; (c) Refute conjectures (or repair them); (d) Suggest conjectures (or sharpen existing ones); (e) Suggest lines of proof.

The basic idea is to address all those tasks through heuristic search of one or a family of extremal graphs. This can be done in a unified way, i.e., for any formula on one or several invariants and subject to constraints, with the Variable Neighborhood Search (VNS) metaheuristic of Mladenović and Hansen (1997) and Hansen and Mladenović (2001). Given a formula, VNS first searches a local minimum on the family of graphs with possibly some parameters fixed such as the number of vertices n or the number of edges m. This is done by making elementary changes in a greedy way (i.e., decreasing most the objective, in case of minimization) on a given initial graph: rotation of an edge (changing one of its endpoints), removal or addition of one edge, short-cut (i.e., replacing a 2-path by a single edge) detour (the reverse of the previous operation), insertion or removal of a vertex and the like. Once a local minimum is reached, the corresponding graph is perturbed increasingly, by choosing at random another graph in a farther and farther neighborhood. A descent is then performed from this perturbed graph. Three cases may occur: (i) one gets back to the unperturbed local optimum, or (ii) one gets to a new local optimum with an equal or worse value than the unperturbed one, in which case one moves to the next neighborhood, or (iii) one gets to a new local optimum with a better value than the unperturbed one, in which case one recenters the search there. The neighborhoods for perturbation are usually nested and obtained from the unperturbed graph by addition, removal or moving of $1, 2, \ldots, k$ edges.

Refuting conjectures given in inequality form, i.e., $i_1(G) \leq i_2(G)$ where i_1 and i_2 are invariants, is done by minimizing the difference between right and left hand sides; a graph with a negative value then refutes the conjectures. Obtaining new conjectures is done from values of invariants for a family of (presumably) extremal graphs depending on some parameter(s) (usually n and/or m). Three ways are used (Caporossi and Hansen, 2004): (i) a *numerical way*, which exploits the mathematics of Principal Component Analysis to find a basis of affine relations between graph invariants satisfied by those extremal graphs considered; (ii) a *geometric way*, i.e., finding with a "gift-wrapping" algorithm the convex hull of the set of points corresponding to the extremal graph in invariants space: each facet then gives a linear inequality; (iii) an *algebraic way*, which consists in determining the class to which all extremal graphs belong, if there is one (often it is a simple one such as paths, stars, complete graphs, etc); then formulae giving the value of individual invariants in function of n and/or m are combined. Obtaining possible lines of proof is done by checking if one or just a few of the elementary changes always suffice to get the extremal graphs found; if so, one can try to show that it is possible to apply such changes to any graph of the class under study.

Recall that the Laplacian matrix $L(G)$ of a graph $G = (V, E)$ is the difference of a diagonal matrix with values equal to the degrees of vertices of G, and the adjacency matrix of G. The algebraic connectivity of G is the second smallest eigenvalue of the Laplacian matrix (Fiedler, 1973). In this paper, we apply AGX to get structural conjectures for graphs with minimum and maximum algebraic connectivity given their order $n = |V|$ and size $m = |E|$, as well as implied bounds on the algebraic connectivity.

The paper is organized as follows. Definitions, notation and basic results on algebraic connectivity are recalled in the next section. Graphs with minimum algebraic connectivity are studied in Section 3; it is conjectured that they are path-complete graphs (Harary, 1962; Soltès, 1991); a lower bound on $a(G)$ is proved for one family of such graphs. Graphs with maximum algebraic connectivity are studied in Section 4. Extremal graphs are shown to be complements of disjoint triangles, paths P_3, edges K_2 and isolated vertices K_1. A best possible upper bound on $a(G)$ in function of m is then found and proved.

2. Definitions and basic results concerning algebraic connectivity

Consider again a graph $G = \big(V(G), E(G)\big)$ such that $V(G)$ is the set of vertices with cardinality n and $E(G)$ is the set of edges with cardinality m. Each $e \in E(G)$ is represented by $e_{ij} = \{v_i, v_j\}$ and in this case, we say that v_i is *adjacent* to v_j. The *adjacency matrix* $A = [a_{ij}]$ is an $n \times n$ matrix such that $a_{ij} = 1$, when v_i and v_j are adjacent and $a_{ij} = 0$, otherwise. The *degree* of v_i, denoted $d(v_i)$, is the number of edges incident with v_i. The *maximum degree* of G, $\Delta(G)$, is the largest vertex degrees of G. The *minimum degree* of G, $\delta(G)$, is defined analogously. *The vertex* (*or edge*) *connectivity* of G, $\kappa(G)$ (or $\kappa'(G)$) is the minimum number of vertices (or edges) whose removal from G results in a disconnected graph or a trivial one. A *path* from v to w

in G is a sequence of distinct vertices starting with v and ending with w such that consecutive vertices are adjacent. Its length is equal to its number of edges. A graph is connected if for every pair of vertices, there is a *path* linking them. The distance $d_G(v, w)$ between two vertices v and w in a connected graph is the length of the shortest path from v to w. The *diameter* of a graph G, d_G, is the maximum distance between two distinct vertices. A path in G from a node to itself is referred to as a *cycle.* A connected acyclic graph is called a *tree.* A complete graph, K_n, is a graph with n vertices such that for every pair of vertices there is an edge. A *clique* of G is an induced subgraph of G which is complete. The size of the largest clique, denoted $\omega(G)$, is called *clique number.* An empty graph, or a trivial one, has an empty edge set. A set of pairwise non adjacent vertices is called an *independent set.* The size of the largest independent set, denoted $\alpha(G)$, is the independence number. For further definitions see Godsil and Royle (2001).

As mentionned above, the *Laplacian* of a graph G is defined as the $n \times n$ matrix

$$L(G) = \triangle - A, \tag{1.1}$$

when A is the adjacency matrix of G and $\triangle$ is the diagonal matrix whose elements are the vertex degrees of G, called the *degree matrix* of G. $L(G)$ can be associated with a positive semidefinite quadratic form, as we can see in the following proposition:

PROPOSITION 1.1 (MERRIS, 1994) *Let G be a graph. If the quadratic form related to $L(G)$ is*

$$q(x) = xL(G)x^t, \quad x \in \Re^n,$$

then q is positive semidefinite.

The polynomial $p_{L(G)}(\lambda) = \det(\lambda I - L(G)) = \lambda^n + q_1\lambda^{n-1} + \cdots + q_{n-1}\lambda + q_n$ is called the *characteristic polynomial* of $L(G)$. Its *spectrum* is

$$\zeta(G) = (\lambda_1, \ldots, \lambda_{n-1}, \lambda_n), \tag{1.2}$$

where $\forall i$, $1 \leq i \leq n$, λ_i is an eigenvalue of $L(G)$ and $\lambda_1 \geq \ldots \geq \lambda_n$.

According to Proposition 1.1, $\forall i$, $1 \leq i \leq n$, λ_i is a non-negative real number. Fiedler (1973) defined λ_{n-1} as the *algebraic connectivity* of G, denoted $a(G)$.

We next recall some inequalities related to algebraic connectivity of graphs. These properties can be found in the surveys of Fiedler (1973) and Merris (1994).

PROPOSITION 1.2 *Let G_1 and G_2 be spanning graphs of G such that $E(G_1) \cap E(G_2) = \phi$. Then $a(G_1) + a(G_2) \leq a(G_1 \cup G_2)$.*

PROPOSITION 1.3 *Let G be a graph and G_1 a subgraph obtained from G by removing k vertices and all adjacent edges in G. Then*

$$a(G_1) \geq a(G) - k.$$

PROPOSITION 1.4 *Let G be a graph. Then,*
(1) $a(G) \leq [n/(n-1)]\delta(G) \leq 2|E|/(n-1)$;
(2) $a(G) \geq 2\delta(G) - n + 2$.

PROPOSITION 1.5 *Let G be a graph with n vertices and $G \neq K_n$. Suppose that G contains an independent set with p vertices. Then,*

$$a(G) \leq n - p.$$

PROPOSITION 1.6 *Let G be a graph with n vertices. If $G \neq K_n$ then $a(G) \leq n - 2$.*

PROPOSITION 1.7 *Let G be a graph with n vertices and m edges. If $G \neq K_n$ then*

$$a(G) \leq \left(\frac{2m}{n-1}\right)^{(n-1)/n}$$

PROPOSITION 1.8 *If $G \neq K_n$ then $a(G) \leq \delta(G) \leq \kappa(G)$. For $G = K_n$, we have $a(K_n) = n$ and $\delta(K_n) = \kappa(K_n) = n - 1$.*

PROPOSITION 1.9 *If G is a connected graph with n vertices and diameter d_G, then $a(G) \geq 4/nd_G$ and $d_G \leq \sqrt{2\Delta(G)/a(G)}\log_2(n^2)$.*

PROPOSITION 1.10 *Let T be a tree with n vertices and diameter d_T. Then,*

$$a(T) \leq 2\left[1 - \cos\left(\frac{\pi}{d_T + 1}\right)\right].$$

A partial graph of G is a graph G_1 such that $V(G_1) = V(G)$ and $E(G_1) \subset E(G)$.

PROPOSITION 1.11 *If G_1 is a partial graph of G then $a(G_1) \leq a(G)$.*

Moreover

PROPOSITION 1.12 *Consider a path P_n and a graph G with n vertices. Then, $a(P_n) \leq a(G)$.*

Consider graphs $G_1 = \big(V(G_1), E(G_1)\big)$ and $G_2 = \big(V(G_2), E(G_2)\big)$. The *Cartesian product* of G_1 and G_2 is a graph $G_1 \times G_2$ such that $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and $\big((u_1, u_2), (v_1, v_2)\big) \in E(G_1 \times G_2)$ if and only if either $u_1 = v_1$ and $(u_2, v_2) \in E(G_2)$ or $(u_1, v_1) \in E(G_1)$ and $u_2 = v_2$.

PROPOSITION 1.13 *Let G_1 and G_2 be graphs. Then,*

$$a(G_1 \times G_2) = \min\{a(G_1), a(G_2)\}.$$

3. Minimizing $a(G)$

When minimizing $a(G)$ we found systematically graphs belonging to a little-known family, called *path-complete graphs* by Soltès (1991). They were previously considered by Harary (1962) who proved that they are (non-unique) connected graphs with n vertices, m edges and maximum diameter. Soltès (1991) proved that they are the unique connected graphs with n vertices, m edges and maximum average distance between pairs of vertices. Path-complete graphs are defined as follows: they consist of a complete graph, an isolated vertex or a path and one or several edges joining one end vertex of the path (or the isolated vertex) to one or several vertices of the clique, see Figure 1.1 for an illustration. We will need a more precise definition:

For n and $t \in N$ when $1 \le t \le n-2$, we consider a new family of connected graphs with n vertices and $m_t(r)$ edges as follows:

$$G\big(n, m_t(r)\big) = \{G \mid \text{for } t \le r \le n-2,\ G \text{ has } m_t(r) \text{ edges},\\ m_t(r) = (n-t)(n-t-1)/2 + r\}.$$

DEFINITION 1.1 Let $n, m, t, p \in \mathbb{N}$, with $1 \le t \le n-2$ and $1 \le p \le n-t-1$. A graph with n vertices and m edges such that

$$\frac{(n-t)(n-t-1)}{2} + t \le m \le \frac{(n-t)(n-t-1)}{2} + n - 2$$

is called (n, p, t) *path-complete graph*, denoted $\mathrm{PC}_{n,p,t}$, if and only if

(1) the maximal clique of $\mathrm{PC}_{n,p,t}$ is K_{n-t};

(2) $\mathrm{PC}_{n,p,t}$ has a t-path $P_{t+1} = [v_0, v_1, v_2, \ldots, v_t]$ such that $v_0 \in K_{n-t} \cap P_{t+1}$ and v_1 is joined to K_{n-t} by p edges;

(3) there are no other edges.

Figure 1.1 displays a (n, p, t) *path-complete graph.*

It is easy to see that all connected graphs with n vertices can be partitioned into the disjoint union of the following subfamilies:

$$G(n, m_1) \oplus G(n, m_2) \oplus \cdots \oplus G(n, m_{n-2}).$$

Besides, for every (n, p, t), $\mathrm{PC}_{n,p,t} \in G(n, m_t)$.

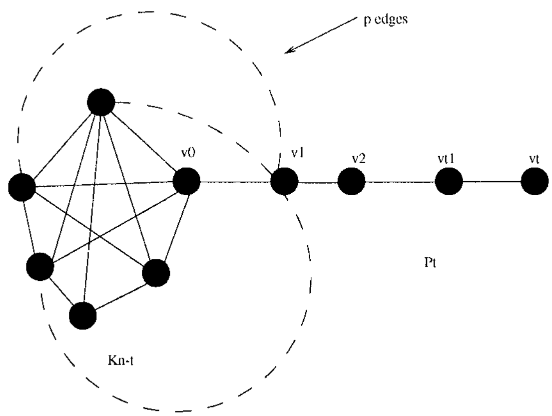
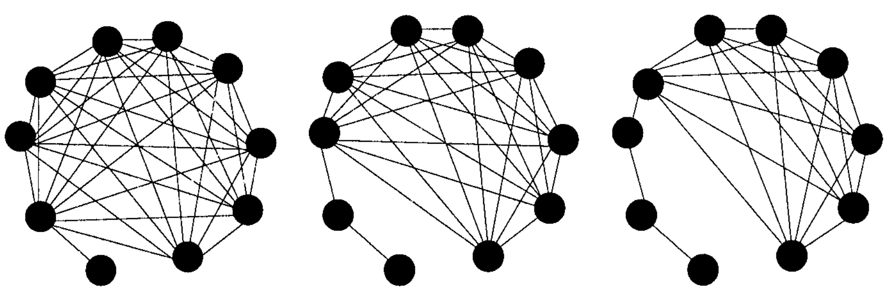


Figure 1.1. A (n, p, t) path-complete graph



$(m = 37;\ a(G) = 1)$ $(m = 30;\ a(G) = 0.435)$ $(m = 24;\ a(G) = 0.256)$

Figure 1.2. Path-complete graphs

3.1 Obtaining conjectures

Using AGX, connected graphs $G \neq K_n$ with (presumably) minimum algebraic connectivity were determined for $3 \leq n \leq 11$ and $n-1 \leq m \leq n(n-1)/2 - 1$. As all graphs turned out to belong to the same family, a structural conjecture was readily obtained.

CONJECTURE 1.1 *The connected graphs $G \neq K_n$ with minimum algebraic connectivity are all path-complete graphs.*

A few examples are given in Figure 1.2, for $n = 10$.

Numerical values of $a(G)$ for all extremal graphs found are given in Table 1.1, for $n = 10$ and $n - 1 \leq m \leq n(n-1)/2 - 1$.

For each n, a piecewise concave function of m is obtained. From this table and the corresponding Figure 1.3 we obtain:

Table 1.1. $n = 10$; $\min a(G)$ on m

m	9	10	11	12	13	14	15	16	17
$a(G)$	0.097	0.103	0.109	0.115	0.123	0.134	0.137	0.151	0.170
m	18	19	20	21	22	23	24	25	26
$a(G)$	0.175	0.177	0.208	0.238	0.247	0.252	0.256	0.345	0.384
m	27	28	29	30	31	32	33	34	35
$a(G)$	0.406	0.419	0.428	0.435	0.673	0.801	0.876	0.924	0.957
m	36	37	38	39	40	41	42	43	44
$a(G)$	0.981	1	2	3	4	5	6	7	8

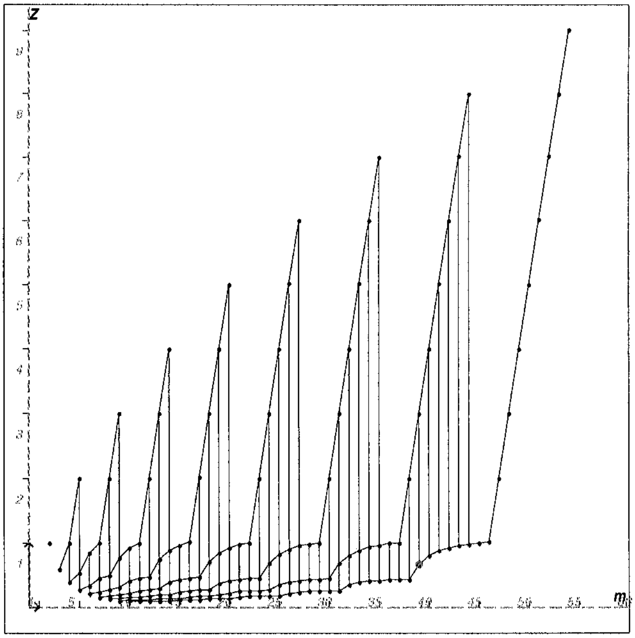


Figure 1.3. $\min a(G)$; $a(G)$ on m

CONJECTURE 1.2 *For each $n \geq 3$, the minimum algebraic connectivity of a graph G with n vertices and m edges is an increasing, piecewise concave function of m. Moreover, each concave piece corresponds to a family $\mathrm{PC}_{n,p,t}$ of path-complete graphs. Finally, for $t = 1$, $a(G) = \delta(G)$, and for $t \geq 2$, $a(G) \leq 1$.*

3.2 Proofs

We do not have a proof of Conjecture 1.1, nor a complete proof of Conjecture 1.2. However, we can prove some of the results of the latter.

We now prove that, under certain conditions, the algebraic connectivity of a path-complete graph minimizes the algebraic connectivity of every graph in $G(n, m_t)$, when $t = 1$ and $t = 2$.

PROPERTY 1.1 *Consider a path-complete graph* $\mathrm{PC}_{n,p,t}$.
(1) *For* $t = 1$, $a(\mathrm{PC}_{n,p,1}) = p$,
(2) *For* $t \geq 2$, $a(\mathrm{PC}_{n,1,t}) \leq a(\mathrm{PC}_{n,p,t}) \leq 1$.

Proof. Let us start with the second statement. According to the definition of path-complete graph, $\delta(R_{n,p,t}) = 1$, when $t \geq 2$. From Propositions 1.8 and 1.11, we obtain the following inequalities

$$a(\mathrm{PC}_{n,1,t}) \leq a(\mathrm{PC}_{n,p,t}) \leq \delta(\mathrm{PC}_{n,p,t}).$$

Therefore, $a(\mathrm{PC}_{n,p,t}) \leq 1$.

Now, consider the first statement. Let $t = 1$ and $\overline{\mathrm{PC}_{n,p,1}}$ be the complement graph of $\mathrm{PC}_{n,p,1}$. Figure 1.4 shows both graphs, $\overline{\mathrm{PC}_{n,p,1}}$ and $\mathrm{PC}_{n,p,1}$.

$\overline{\mathrm{PC}_{n,p,1}}$ has p isolated vertices and one connected component isomorphic to $K_{1,n-p-1}$. Its Laplacian matrix is,

$$L(\overline{\mathrm{PC}_{n,p,1}}) = \begin{bmatrix} L(K_{1,n-p-1}) & 0 \\ 0 & 0 \end{bmatrix}.$$

From Biggs (1993), we have

$$\det[L(K_{1,b}) - \lambda I_{b+1}] = \lambda[\lambda - (b+1)](\lambda - 1)^{b-1}.$$

Then,

$$\begin{aligned} det[L(\overline{\mathrm{PC}_{n,p,1}}) - \lambda I_n] &= (-\lambda)^p \det[L(K_{1,n-p-1}) - \lambda I_{n-p}] \\ &= (-\lambda)^p \lambda[\lambda - (n-p)](\lambda - 1)^{n-p-2}. \end{aligned}$$

According to Merris (1994), if $\zeta(G) = (\lambda_n, \lambda_{n-1}, \ldots, \lambda_2, 0)$ then $\zeta(\overline{G}) = (n - \lambda_2, n - \lambda_3, \ldots, n - \lambda_n, 0)$. So, we have

$$\begin{aligned} \zeta(\overline{\mathrm{PC}_{n,p,1}}) &= (n-p, 1, \ldots, 1, 0, \ldots, 0) \\ \zeta(\mathrm{PC}_{n,p,1}) &= (n, \ldots, n, n-1, \ldots, n-1, p, 0). \end{aligned}$$

Consequently, $a(\mathrm{PC}_{n,p,1}) = p$. □

PROPERTY 1.2 *For* $(n, p, 1)$ *path-complete graphs, we have* $\delta(\mathrm{PC}_{n,p,1}) = \kappa(\mathrm{PC}_{n,p,1}) = p$.

Proof. It follows from Definition 1.1, that $\delta(\mathrm{PC}_{n,p,1}) = p$. Applying Proposition 1.8 we obtain $a(\mathrm{PC}_{n,p,1}) \leq k(\mathrm{PC}_{n,p,1}) \leq p$. Since Property 1.1 gives $a(\mathrm{PC}_{n,p,1}) = p$ then $k(\mathrm{PC}_{n,p,1}) = p$. □

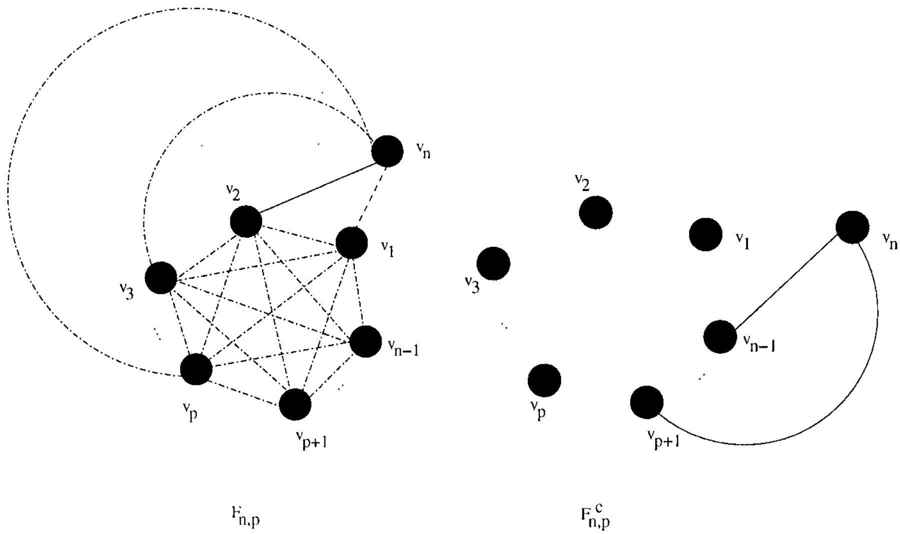


Figure 1.4. $\mathrm{PC}_{n,p,1}$ and its complement $\overline{\mathrm{PC}_{n,p,1}}$

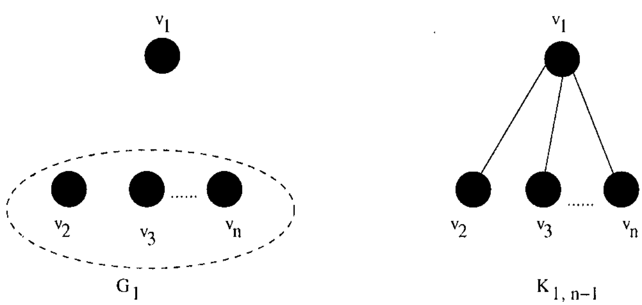


Figure 1.5. Graphs $K_{1,n-1}$ and G_1

PROPOSITION 1.14 *Among all* $G \in G(n, m_1)$ *with maximum degree* $n-1$*,* $a(G)$ *is minimized by* $\mathrm{PC}_{n,1,1}$.

Proof. Let G be a graph with n vertices. Consider spanning graphs of G $K_{1,n-1}$ and G_1 such that $E(K_{1,n-1}) \cap E(G_1) = \phi$ and G_1 has two connected components, one of them with $n-1$ vertices. Figure 1.5 shows these graphs.

We may consider $G = (V, E)$ where $V(G) = V(K_{1,n-1}) = V(G_1)$ and $E(G) = E(K_{1,n-1}) \cup E(G_1)$. Then, $\Delta(G) = n-1$. According to Proposition 1.2, we have $a(K_{1,n-1}) + a(G_1) \leq a(G)$. From Biggs (1993), $a(K_{1,n-1}) = 1$. Since G_1 is a disconnected graph then $a(G_1) = 0$. However, $a(\mathrm{PC}_{n,1,1}) = 1$, therefore $a(G) \geq 1$. $\square$

PROPOSITION 1.15 *For every $G \in G(n, m_1)$ such that $\delta(G) \geq (n-2)/2 + p/2$, where $1 \leq p \leq n-2$, we have*

$$a(G) \geq a(\mathrm{PC}_{n,p,1}) = p.$$

Proof. Consider $G \in G(n, m_1)$ with $\delta(G) \geq (n-2)/2 + p/2$. According to Proposition 1.4, we have

$$a(G) \geq 2\delta(G) - n + 2 \geq 2\left\lceil \frac{n-2}{2} + \frac{p}{2} \right\rceil - n + 2 = p.$$

Consequently, $a(G) \geq a(\mathrm{PC}_{n,p,1}) = p$. □

PROPOSITION 1.16 *For every $G \in G(n, m_2)$ such that $\delta(G) \geq (n-1)/2$, we have*

$$a(G) \geq 1 \geq a(\mathrm{PC}_{n,p,2}).$$

Proof. Consider $G \in G(n, m_2)$ with $\delta(G) \geq (n-1)/2$. According to Proposition 1.4, we have

$$a(G) \geq 2\delta(G) - n + 2 \geq 2\left\lceil \frac{n-1}{2} \right\rceil - n + 2 = 1.$$

From Property 1.1, $a(\mathrm{PC}_{n,p,2}) \leq 1$. Then, $a(G) \geq 1 \geq a(\mathrm{PC}_{n,p,2})$. □

To close this section we recall a well-known result.

PROPOSITION 1.17 *Let T be a tree with n vertices. For every T, $a(T)$ is minimized by the algebraic connectivity of a single path P_n, where $a(P_n) = 2[1 - \cos(\pi/n)]$. Moreover, for every graph G with n vertices $a(P_n) \leq a(G)$.*

4. Maximizing $a(G)$

4.1 Obtaining conjectures

Using AGX, connected graphs $G \neq K_n$ with (presumably) maximum algebraic connectivity $a(G)$ were determined for $3 \leq n \leq 10$ and $(n-1)(n-2)/2 \leq m \leq n(n-1)/2 - 1$. We then focused on those among them with maximum $a(G)$ for a given m. These graphs having many edges, it is easier to understand their structure by considering their complement $\overline{G}$. It appears that these $\overline{G}$ are composed of disjoint triangles K_3, paths P_3, edges K_2 and isolated vertices K_1.

A representative subset of these graphs $\overline{G}$ is given in Figure 1.6.

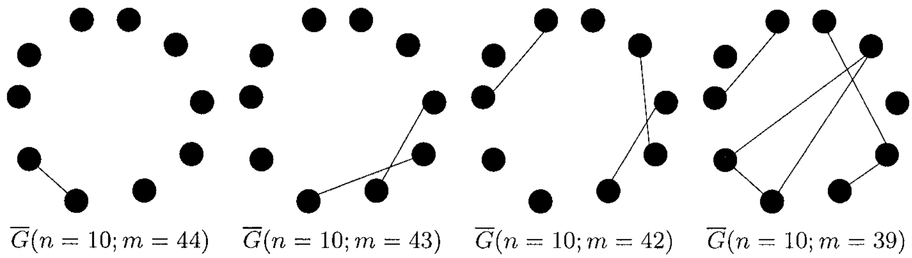


Figure 1.6.

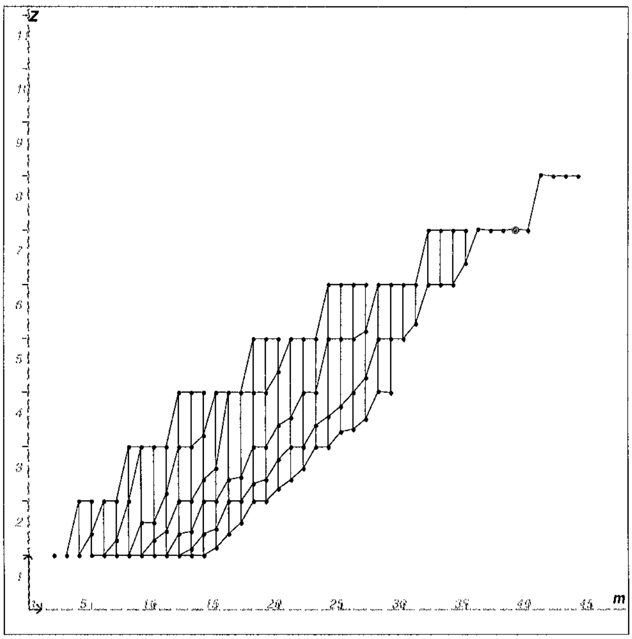


Figure 1.7. $\max a(G)$; $a(G)$ on m

CONJECTURE 1.3 *For all $m \geq 2$ there is a graph $G \neq K_n$ with maximum algebraic connectivity $a(G)$ the complement $\overline{G}$ of which is the disjoint union of triangles K_3, paths P_3, edges K_2 and isolated vertices K_1.*

Values of $a(G)$ for all extremal graphs obtained by AGX are represented in function of m in Figure 1.7.

It appears that the maximum $a(G)$ follow an increasing "staircase" with larger and larger steps. Values of $a(G)$, m and n for the graphs of this staircase (or upper envelope) are listed in Table 1.2.

An examination of Table 1.2 leads to the next conjecture.

Table 1.2. Value of $a(G)$, m and n for graphs, with maximum $a(G)$ for m given, found by AGX

$a(G)$	.	1	1	2	2	2	2	3	3	3	3	4	4	4	4	4	4	5	5	5	5	5
m	.	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
n	.	3	4	4	4	5	5	5	5	6	6	6	6	6	7	7	7	7	7	7	7	7

$a(G)$	5	6	6	6	6	6	6	6	6	7	7	7	7	7	7	7	7	8	8	8	8	8
m	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44
n	8	8	8	8	8	8	8	9	9	9	9	9	9	9	9	10	10	10	10	10	10	10

CONJECTURE 1.4 *For all $n \geq 4$ there are $n-1$ consecutive values of m (beginning at 3) for which a graph $G \neq K_n$ with maximum algebraic connectivity $a(G)$ has n vertices. Moreover, for the first $\lfloor (n-1)/2 \rfloor$ of them $a(G) = n-2$ and for the last $\lceil (n-1)/2 \rceil$ of them $a(G) = n-3$.*

Considering the successive values of $a(G)$ for increasing m, it appears that for $a(G) = 2$ onwards their multiplicities are 4, 4, 6, 6, 8, 8, ... After a little fitting, this leads to the following observation:

$$\left\lceil \frac{a(G)(a(G)+2)}{2} \right\rceil \leq m$$

and to our final conjecture:

CONJECTURE 1.5 *If G is a connected graph such that $G \neq K_n$ then*

$$a(G) \leq \lfloor -1 + \sqrt{1+2m} \rfloor$$

and this bound is sharp for all $m \geq 2$.

One can easily see that this conjecture improves the bound already given in Proposition 1.7, i.e., $a(G) \leq \big(2m/(n-1)\big)^{(n-1)/n}$.

4.2 Proofs

We first prove Conjectures 1.3 and 1.4. Then, we present a proof for the last conjecture. The extremal graphs found point the way.

Proof of Conjectures 1.3 and 1.4. From Propositions 1.6 and 1.8 if $G \neq K_n$, $a(G) \leq \delta(G) \leq n-2$. For this last bound to hold as an equality one must have $\delta(G) = n-2$, which implies G must contain all edges except up to $\lfloor n/2 \rfloor$ of them, i.e., $n(n-1)/2 - \lfloor n/2 \rfloor \leq m \leq n(n-1)/2 - 1$. Moreover, the missing edges of G (or edges of $\overline{G}$) must form a matching. Assume there are $1 \leq r \leq \lfloor n/2 \rfloor$ missing edges and that they form a matching. Then from Merris (1994) $\det[L(\overline{G})-\lambda I_n] = -\lambda^{n-2r}\lambda^r(\lambda-2)^r$. Hence

$$\zeta(\overline{G}) = (\underbrace{2,\ldots,2}_{r \text{ times}},0,\ldots,0), \quad \zeta(G) = (\underbrace{n,\ldots,n}_{n-r-1 \text{ times}},\underbrace{n-2,\ldots,n-2}_{r \text{ times}},0)$$

and $a(G) = n-2$. If there are $r > \lfloor n/2 \rfloor$ missing edges in G, $a(G) \le \delta(G) \le n-3$. Several cases must be considered to show that this bound is sharp, in all of which $r \le n$, as otherwise $\delta(G) < n-3$. Moreover, one may assume $r \le n-1$ or otherwise there is a smaller n such that all edges can be used and with $\delta(G)$ as large or larger:

(i) $r \bmod 3 = 0$. Then there is a $t \in \mathbb{N}$ such that $r = 3t$. Assume the missing edges of G form disjoint triangles in $\overline{G}$. Then (Biggs, 1993)

$$\det[L(K_3) - \lambda I_3] = \lambda(\lambda-3)^2$$

and

$$\det[L(\overline{G}) - \lambda I_n] = (-\lambda)^{n-r}\lambda^t(\lambda-3)^{2t}.$$

Hence

$$\zeta(\overline{G}) = (\underbrace{3,\ldots,3}_{2t \text{ times}},0,\ldots,0),$$

$$\zeta(\overline{G}) = (\underbrace{n,\ldots,n}_{n-2t-1 \text{ times}},\underbrace{n-3,\ldots,n-3}_{2t \text{ times}},0)$$

and $a(G) = n-3$.

(ii) $r \bmod 3 = 1$. Then there is a $t \in \mathbb{N}$ such that $r = 3t+1$. Assume the missing edges of G form t disjoint triangles and a disjoint edge. Then, as above,

$$\det[L(\overline{G}) - \lambda I_n] = (-\lambda)^{n-r-1}\lambda^{(r+2)/3}(\lambda-2)(\lambda-3)^{(2r-2)/3},$$

and $a(G) = n-3$.

(iii) $r \bmod 3 = 2$. Then there is a $t \in \mathbb{N}$ such that $r = 3t+2$. Assume the missing edges of G form t disjoint triangles and a disjoint path P_3 with 2 edges. From the characteristic polynominal of $L(P_3)$ and similar arguments as above one gets $a(G) = n-3$. □

Proof of Conjecture 1.5. Let $S \neq K_n$ a graph with all edges except up to $\lfloor n/2 \rfloor$ of them. So, $n(n-1)/2 - \lfloor n/2 \rfloor \le m \le n(n-1)/2 - 1$.

(i) If n is odd then,

$$\frac{n(n-1)}{2} - \frac{n-1}{2} \le m \le \frac{n(n-1)}{2} - 1.$$

Since $n^2 - 2n + 1/2 \geq n(n-2)/2$, $m \geq n(n-2)/2$.

(ii) If n is even, then

$$\frac{n(n-1)}{2} - \frac{n}{2} \leq m \leq \frac{n(n-1)}{2} - 1.$$

So, $2m \geq n(n-2)$ and $n-2 \leq \lfloor -1 + \sqrt{1+2m} \rfloor$. From Proposition 1.6, $a(G) \leq n-2$. Then, $a(G) \leq \lfloor -1 + \sqrt{1+2m} \rfloor$.

Now, consider $(n-1)(n-2)/2 \leq m \leq n(n-1)/2 - (\lfloor n/2 \rfloor + 1)$. This way, $m = n(n-1)/2 - r$, with $\lfloor n/2 \rfloor + 1 \leq r \leq n-1$. So, $r \leq \frac{3}{2}(n-1)$. We can add n^2 to each side of the inequality above. After some algebraic manipulations, we get $(n-2)^2 \leq 2m+1$. So, $n-3 \leq -1 + \sqrt{2m+1}$.

From the proof of Conjecture 1.4, we have $a(S) \leq n-3$. Then, $a(S) \leq \lfloor -1 + \sqrt{1+2m} \rfloor$. As we can consider every $G \neq K_n$ with n vertices as a partial (spanning) graph of S, from Proposition 1.11, we then have $a(G) \leq a(S) \leq \lfloor -1 + \sqrt{1+2m} \rfloor$. □

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