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ON CONNECTED GRAPHS WITH MAXIMAL INDEX

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Abstract. Let $\mathcal{H}(n, n+k)$ denote the set of all connected graps having n vertices and $n+k$ edges ($k \geq 0$). The graphs in $\mathcal{H}(n, n+k)$ with maximal index are determined (i) for certain small values of n and k, (ii) for arbitrary fixed k and large enough n. The results include a proof of a conjecture of Brualdi and Solheid [1].

1. Introduction and some numerical results

We consider only finite undirected graphs without loops or multiple edges. The largest eigenvalue of a $(0, 1)$-adjacency matrix of a graph G is called the *index* of G. The importance of this algebraic invariant was recognized at an early stage in the development of graph spectra: in the fundamental paper [2], for example, Collatz and Sinogowitz studied the ordering of graphs by their indices. They established that among trees with n vertices, the star $K_{1,n-1}$ has maximal index and the path P_n has minimal index. They also raised the question of finding the most irregular graph with a given number of vertices: here the proposed measure of irregularity is $\delta = \rho - \bar{d}$, where ρ denotes index and $\bar{d}$ the average depree. (Thus $\delta \geq 0$, with equality precisely for regular graphs [3, Theorem 3.8].) Using their tables of spectra of graphs with up to 5 vertices, Collatz and Sinogowitz showed that among graphs with n vertices $n \leq 5$, the most irregular graph is $K_{1,n-1}$. In general, however the most irregular graphs have not been characterized. We present some computational results which show that stars are not always the most irregular among graphs with a given number of vertices.

The six-vertex graphs G_1 and G_2 shown in Fig. 1 have indices $\rho_1 = \sqrt{5}$ and $\rho_2 \approx 2.56$ respectively. Since $\bar{d} = 5/3$ for both graphs, the graph G_2 is more irregular than the star G_1.

Restricting the question to connected graphs, we find that still the star is not necessarily the most irregular connected graph with a given number of vertices. The following example was found using the expert system "Graph" [5]. Let $G_1 = K_{1,24}$

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and let G_2 be obtained from the complete graph K_6 by adding 19 pendant edges at a single vertex. We have $\rho_1 = \sqrt{244} \approx 4.8990$, $\rho_2 \approx 5.8837$, $\bar{d}_1 = 1.92$ and $\bar{d}_2 = 2.72$. Hence $\delta_1 \approx 2.9790$ and $\delta_2 \approx 3.1637$: in particular, $\delta_2 > \delta_1$.

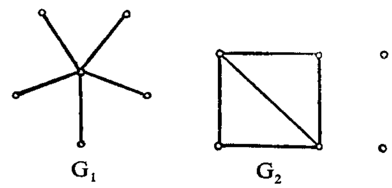

Fig. 1

Among graphs with both a given number of vertices and a given number of edges, the most irregular graphs are precisely those with maximal index. Following the notation of [1], let $\mathcal{H}(n, e)$ denote the set of connected graphs with n vertices and e edges. For $n > 1$, $k \geq 0$ let $G_{n,k}$ be the graph in $\mathcal{H}(n, n+k)$ which is of the form shown in Fig. 2 with p chosen as large as possible.

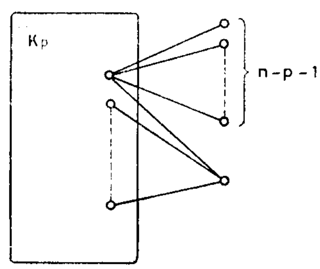

Fig. 2

Inspection of the connected graphs with up to 7 vertices leads one to speculate that $G_{n,k}$ (and $G_{n,k}$ alone) has the largest index of any graph in $\mathcal{H}(n, n+k)$. (Data from "Graph" for the 853 connected graphs on 7 vertices are tabulated in [4]). Simić [8, 9] proved that this is indeed true for unicyclic and bicyclic graphs (the cases $k = 0$, $k = 1$ respectively). Brualdy and Solheid [1] showed independently of Simić that $G_{n,k}$ is the unique graph of maximal index in $\mathcal{H}(n, n+h)$ when $k = 0, 1, 2$; but they found counterexamples for $k = 3, 4, 5$, namely the graphs $H_{n,k}^{(i)} (k = 3, 4, 5)$ of Fig. 3. For each $k \in \{3, 4, 5\}$ the graphs $H_{n,k}^{(i)}$ in Fig. 3 represent an exhaustive list of candidates for graphs in $\mathcal{H}(n, n+k)$ having maximal index [1, Theorem 2.1]. Note that $N_{n,k}^{(k-1)} = G_{n,k}$ $(k = 3, 4, 5)$, and that $H_{n,4}^{(2)}$ is reproduced with a superfluous edge in [1, Figure 10]. The following results were obtained using the system "Graph" to carry out the calculations.

We have $\rho(H_{n,3}^{(1)}) < \rho(H_{n,3}^{(2)})$ for $7 \leq n \leq 24$, while $\rho(H_{25,3}^{(1)}) > \rho(H_{25,3}^{(2)})$. Further, $\rho(H_{n,4}^{(2)}) < \rho(H_{n,4}^{(1)}) < \rho(H_{n,4}^{(3)})$ for $\beta \leq n \leq 36$ and $\rho(H_{n,5}^{(3)}) < \rho(H_{n,5}^{(1)}) <$

$\rho(H_{n,5}^{(2)}) < \rho(H_{n,5}^{(4)})$ for $9 \leq n \leq 15$ while $\rho(H_{n,5}^{(5)}) < \rho(H_{n,5}^{(2)}) < \rho(H_{n,5}^{(1)}) < \rho(H_{n,5}^{(4)})$ for $16 \leq n \leq 38$. For large enough n, however, it is known that when $k \in \{3,4,5\}$, $H_{n,k}^{(1)}$ is the unique graph with maximal index in $\mathcal{H}(n, n+k)$ [1, Theorem 3.3].

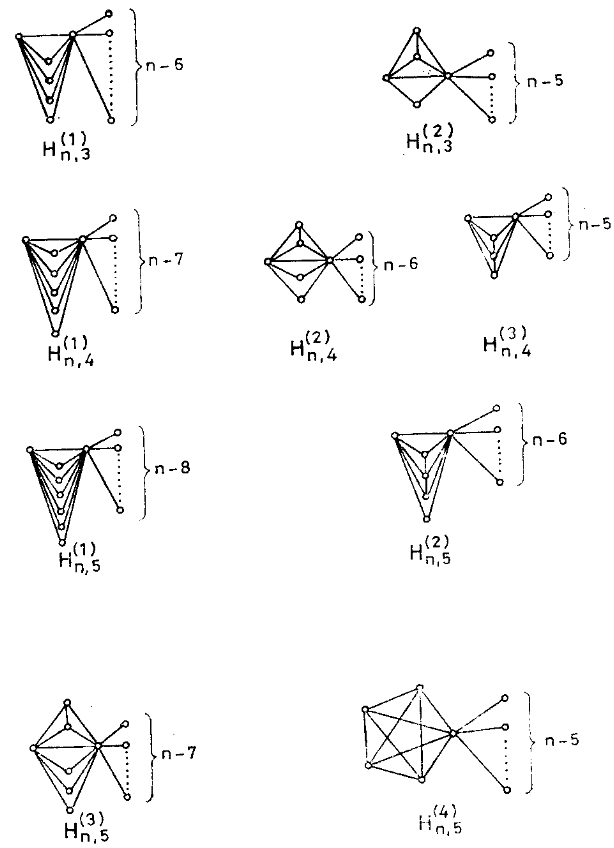

Fig. 3 Some graphs $H_{n,k}^{(i)}$ in $\mathscr{H}(n, n+k)$ ($k = 3, 4, 5$)

Now consider a star $K_{1,n-1}$ ($n \geq 3$) having vertices $1, 2, \ldots, n$, with vertex 1 as the central vertex. For $1 \leq k \leq n-3$, let $H_{n,k}$ be the graph obtained from $K_{1,n-1}$ by joining vertex 2 to vertices $3, 4, \ldots, k+3$. Thus $H_{n,k} = H_{n,k}^{(1)}$ for $k \in \{3,4,5\}$. Brualdi and solheid [1] conjectured that for fixed $k \neq 2$ and for n sufficiently large, $H_{n,k}$ is the unique graph in $\mathcal{H}(n, n+k)$ whith maximal index. The remainder of this paper is devoted to a proof of this conjecture.

2. Proof of the main result

Let $\mathcal{S}(n, e)$ denote the set of adjacency matrices of graphs with n vertices and e edges, and let $\mathcal{S}^*(n, e)$ be the subset of $\mathcal{S}(n, e)$ consisting of those matrices $A = (a_{ij})$ satisfying

(*) if $i < j$ and $a_{ij} = 1$ then $a_{hk} = 1$ whenever $h < k \leq j$ and $h \leq i$.

A matrix which lies in $\mathcal{S}^*(n, e)$ for some n,e is called a *stepwise* matrix. Brualdi and Solheid [1] show that a graph in $\mathcal{H}(n, e)$ with maximal index has an adjacency matrix $A \in \mathcal{S}(n, e)$: note that $A = (a_{ij})$ where $a_{12} = \cdots = a_{1n} = 1$. In A has spectral radius ρ then, from the theory of irreducible non-negative matrices [6, Chapter XIII], there exists a unique positive unit eigenvector x such that $Ax = \rho x$. Moreover it is straightforward to check that, since A is a stepwise matrix, $x = (x_1, \dots, x_n)^T$ where $x_1 \geq x_2 \geq \cdots \geq x_n$ [7, Lemma 1], a fact which will be used implicitly in what follows.

Note that $H_{n,k}$ has a stepwise adjacency matrix. The same is true of the graph $F_{n,s}$ $(n > s > 2)$ defined as follows: $F_{n,s}$ is obtained from the complete graph K_s by adding $n - s$ vertices adjacent to a single vertex of K_s. We start by showing that for fixed s and large enough n, the index of $F_{n,s}$ is less then $\sqrt{n}$.

LEMMA. *If $n > s^2(s-2)^2$ then $\rho(F_{n,s}) < \sqrt{n}$.*

Proof. Let A be a stepwise adjacency matrix of $F_{n,s}$, let $\rho = \rho(F_{n,s})$ and let $(x_1, x_2, \dots, x_n)^T$ be an eigenvector of A corresponding to ρ. Then $x_2 = \cdots = x_s$, $x_{s+1} = \cdots = x_n$ and we have

$$\rho x_1 = (s-1)x_2 + (n-s)x_n,$$
$$\rho x_2 = x_1 + (s-2)x_2, \;\; \rho x_n = x_1.$$

It follows that ρ is the largest root of $h(x)$, where $h(x) = x^3 - (s-2)x^2 - (n-1)x + (n-s)(s-2)$. It is straightforward to check that when $n > s^2(s-2)^2$ we have $h(\sqrt{n}) > 0$, $h'(\sqrt{n}) > 0$ and $h''(x) > 0$ for all $x \geq \sqrt{n}$. Hence if $n > s^2(s-2)^2$, we have $h(x) > 0$ for all $x \geq \sqrt{n}$ and the result follows.

THEOREM. *For $k > 2$ there exists $N(k)$ such that for $n > N(k)$, $H_{n,k}$ is the unique graph in $\mathcal{H}(n, n+k)$ with maximal index.*

Proof. Let $H_{n,k}$ have adjacency matrix $A' \in \mathcal{S}^*(n, n+k)$ and let $A = (a_{ij})$ be any matrix other than A' in $\mathcal{S}^*(n, n+k)$ with $a_{12} = \cdots = a_{1n} = 1$. Let t be maximal such that $a_{2t} = 1$. Note that t may take any valug between t_0 and $k+2$ inclusive, where $\binom{t_0-2}{2} < k+1 \leq \binom{t_0-1}{2}$. Let $r = k+3-t$ and let ρ, ρ' be the spectral radii of A, A' respectively. In view of [1, Theorem 2.1] it suffices to prove that $\rho' > \rho$ for large enough n. In order to apply the Lemma with $s = k+3$ we assume that $n > (k+3)^2(k+1)^2$: then $\rho < \sqrt{n}$ and $\rho' < \sqrt{n}$ since each of A and A' is the adjacency matrix of a spanning subgraph of $F_{n,k+3}$. Let x, x' be the unique positive unit eigenvectors of A, A' corresponding to ρ, ρ' respectively, say $x = (x_1, \dots, x_n)^T$ and $x' = (x'_1, \dots, x'_n)^T$. Then $x^T x' > 0$ and $x^T x'(\rho' - \rho) = x^T(A' - A)x' = \alpha - \beta$ where $\alpha = x_2(x'_{t+1} + \cdots + x'_{k+3}) + x'_2(x_{t+1} + \cdots + x_{k+3})$ and β is the sum of r terms $x_i x'_j + x'_i x_j$ for which $3 \leq i < j$. Since $x'_3 = \cdots = x'_{k+3}$ and $x_{t+1} = \cdots = x_n$, we have $\alpha = r(x_2 x'_3 + x'_2 x_n)$, while $\beta \leq r(x_3 x'_4 + x'_3 x_4) = r x'_3(x_3 + x_4)$. Consequently it suffices to prove that

(**) $x'_2 x_n > x'_3(x_3 + x_4 - x_2)$ for large enough n.

We now distinguish two cases: (A) $t < k+2$, (B) $t = k+2$. We first prove $(**)$ in case (A) by showing that $x_2'x_n > x_3'x_2$ for large enough n. Since $(\rho'+1)x_2' = x_1' + x_2' + \cdots + x'_{k+3}$ and $(\rho'+1)x_3' = x_1' + x_2' + x_3'$, we have

$$\frac{x_2'}{x_3'} = 1 + \frac{kx_3'}{x_1' + x_2' + x_3'} = 1 + \frac{k}{\rho'+1} > k + \frac{k}{\sqrt{n}+1}.$$

On the other hand, since $\rho x_2 = x_1 + x_3 + \cdots + x_t$ and $\rho x_n = x_1$ we have $\frac{x_2}{x_n} < 1 + (t-2)\frac{x_2}{x_1}$. Accordinagly it suffices to show that $\frac{k}{\sqrt{n+1}} > (t-2)\frac{x_2}{x_1}$ for large enough n. The number of non-zero entries in rows $2, \ldots, t$ of A is $(t-1) + 2(k+1)$ and so $\rho(x_2 + x_3 + \cdots + x_t) < (2k+t+1)x_1$. Hence

$$\begin{aligned}\frac{x_1}{x_2} = \frac{x_1 + \cdots + x_n}{x_1 + \cdots + x_t} &= 1 + \frac{(n-t)x_1}{\rho(x_1 + \cdots + x_t)} \geq 1 + \frac{n-t}{\rho + 2k + t + 1} \\ &\geq 1 + \frac{n-t}{\sqrt{n} + 2k + t + 1}\end{aligned}$$

Therefore, $\frac{x_2}{x_1} \leq \frac{\sqrt{n}+2k+t+1}{\sqrt{n}+2k+n+1}$ and it suffices to prove that $\frac{k}{\sqrt{n}+1} > (t-2)\frac{\sqrt{n}+2k+t+1}{\sqrt{n}+2k+n+1}$ for large enough n. This last inequality has the form $(k+2-t)n > A(k,t)\sqrt{n} + B(k,t)$ and so there exists $M(k,t)$ such that $\rho' > \rho$ whenever $n > M(k,t)$.

Turning now to case (B), we note that here there is just one possibility for A and we have $x_3 = x_4$, $x_5 = \cdots = x_{k+2}$, $x_{k+3} = \cdots = x_n$. Moreover,

$$\begin{aligned}\rho x_1 &= \quad\;\; + x_2 + 2x_3 + (k-2)x_5 + (n-k-2)x_n, \\ \rho x_2 &= x_1 + \quad\;\; + 2x_3 + (k-2)x_5, \\ \rho x_3 &= x_1 + x_2 + \;\; x_3, \\ \rho x_5 &= x_1 + x_2, \\ \rho x_n &= x_1.\end{aligned}$$

In order to prove $(**)$ we show that $x_2'/x_3' > (2x_3 - x_2)/x_n$ for large enough n. As before, $x_2'/x_3' > 1 + k/(\sqrt{n}+1)$. Now

$$\frac{2x_3 - x_2}{x_n} = \frac{2(x_1 + x_2 + x_3) - x_1 - 2x_3 - (k-2)x_5}{x_1} = 1 + \frac{2x_2 - (k-2)x_5}{x_1} \text{ and}$$

$$\begin{aligned}\frac{2x_2 - (k-2)x_5}{x_1} &= \frac{2x_1 + 4x_3 + 2(k-2)x_5 - (k-2)(x_1 + x_2)}{\rho x_1} \\ &< \frac{4x_1 + 4x_2 - (k-2)(x_1 + x_2)(1 - 2/\rho)}{\rho x_1}\end{aligned}$$

By [1, Theorem 3.3] the Theorem holds for $k \leq 5$ and so we assume that $k \geq 6$. Then $\frac{2x_2 - (k-2)x_5}{x_1} < \frac{8(x_1+x_2)}{\rho^2 x_1} \leq \frac{16}{\rho^2}$. Now $\rho > \sqrt{n-1}$ because A is the adjacency matrix of a graph with a star as a proper spanning subgraph, and so it suffices to prove that $k/(\sqrt{n}+1) > 16/(n-1)$ for large enough n. This is clear: indeed the inequality holds for all n under consideration, namely when $k \geq 6$ and $n >$

$(k+3)^2(k+1)^2$. Let $M(k,k+2) = (k+3)^2(k+1)^2$. The theorem is now proved, with $N(k) = \max_{t_0 \le t \le k+2} M(k,t)$ when $k \ge 6$.

Remark. Following [1], let $\mathcal{H}^*(n,e)$ denote the set of of all graphs in $\mathcal{H}(n,e)$ which have a stepwise adjacency matrix. The foregoing arguments show that for $k > 2$, there exists $N(k)$ such that whenever $n > N(k)$ we have $\sqrt{n-1} < \rho(G) < \sqrt{n}$ for all graphs $G \in \mathcal{H}^*(n, n+k)$.

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