On the Maximal Index of Connected Graphs

F. K. Bell
Department of Mathematics
University of Stirling
Stirling FK9 4LA, Scotland

Submitted by Richard A. Brualdi

ABSTRACT

Let $\mathscr{H}(n, e)$ denote the set of all connected graphs having n vertices and e edges. The graphs in $\mathscr{H}(n, n+k)$ with maximal index are determined for k of form $\binom{r}{2} - 1$ and n arbitrary.

1. INTRODUCTION

The graphs we consider are finite, undirected, and without loops or multiple edges. The *index* (or *spectral radius*) of a graph G is the largest eigenvalue of a $(0,1)$ adjacency matrix A of G, and we denote it by $\rho(G)$. Let $\mathscr{G}(n, e)$ be the set of all graphs with n vertices and e edges, and let $\mathscr{H}(n, e)$ be the set of all connected graphs in $\mathscr{G}(n, e)$. The problem of finding the graphs in $\mathscr{G}(n, e)$ with maximal index was solved by Brualdi and Hoffman [1] in the case when

$$e = \binom{d}{2} \qquad \text{for some } d.$$

Further special cases were dealt with by Friedland [5, 6], who also proved an asymptotic result, and the problem was solved for all remaining values of e by Rowlinson [9]. However, the corresponding problem for $\mathscr{H}(n, e)$ has been solved only in certain cases. When e has its minimum value $n-1$, the set $\mathscr{H}(n, e)$ consists of all n-vertex trees, and it was shown by Lovász and

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Pelikán [8] that the star $K_{1,n-1}$ has maximal index. (See also Collatz and Sinogowitz [3].)

In order to discuss the other results known for $\mathscr{H}(n,e)$ we follow [4] in writing $e=n+k$ $(k \geqslant 0)$ and defining graphs $G_{n,k}$ and $H_{n,k}$. Both of these lie in $\mathscr{H}(n,n+k)$, and both have the star $K_{1,n-1}$ as a spanning subgraph. In $G_{n,k}$ the $k+1$ edges not forming part of the spanning star are such that $G_{n,k}$ has as large a complete subgraph as possible. To be precise, let d be the largest integer such that

$$\binom{d-1}{2} \leqslant k+1,$$

and denote by $F_{n,d}$ the graph obtained from the complete graph K_d on d vertices by adding $n-d$ pendant edges at one of its vertices. (Note that $d \leqslant n$ and $F_{n,n}$ is just K_n.) In the case when

$$\binom{d-1}{2} = k+1$$

we define $G_{n,k}$ to be the graph $F_{n,d}$. In all other cases we can write (uniquely)

$$k+1=\binom{d-1}{2}+t \qquad \text{with} \quad 4 \leqslant d \leqslant n-1 \text{ and } 1 \leqslant t \leqslant d-2;$$

then $G_{n,k}$ is defined to be the graph obtained from $F_{n,d}$ by joining a vertex of degree 1 to t vertices of degree $d-1$. The graph $H_{n,k}$ is defined only for $k \leqslant n-3$: it is the graph obtained from the star $K_{1,n-1}$ by joining a vertex of degree 1 to $k+1$ other vertices of degree 1. Note that $G_{n,k}$ and $H_{n,k}$ coincide if and only if $k=0$ or 1.

The graph of maximal index in $\mathscr{H}(n,e)$ is known when

$$\binom{n-1}{2} < e \leqslant \binom{n}{2},$$

because the graph of maximal index in $\mathscr{G}(n,e)$ is then connected (see [9]); it is in fact $G_{n,e-n}$. Brualdi and Solheid [2] considered those cases in which $e=n+k$ with $k \leqslant 5$. They showed that, when $k=0$, 1, or 2, $G_{n,k}$ is the unique graph of maximal index in $\mathscr{H}(n,n+k)$; whereas when $k=3$, 4, or 5, while $G_{n,k}$ has maximal index for some small values of n, it is $H_{n,k}$ which has maximal index for all sufficiently large values of n. These results were extended by Cvetković and Rowlinson in [4]. They proved that, for any fixed $k \geqslant 6$, $H_{n,k}$ is the unique graph of maximal index for all sufficiently large n.

These known results prompt two questions. For an arbitrary fixed $k \geqslant 6$, does $G_{n,k}$ have maximal index in $\mathscr{H}(n, n+k)$ for "small" values of n? And are there values of n and k for which neither of $G_{n,k}$ and $H_{n,k}$ has maximal index? In Section 3 of this paper we provide precise answers to these questions whenever $k+1$ is equal to $\binom{d-1}{2}$ for some $d > 4$. This case is analogous to the basic case $e = \binom{d}{2}$ for $\mathscr{G}(n, e)$ considered by Brualdi and Hoffman, as can be seen by considering the adjacency matrices involved. A solution to the maximal index problem in this case is a natural first step towards understanding the general situation. We show that there is a "transition value" $g(d)$ for n: if $n \leqslant g(d)$ then $G_{n,k}$ has maximal index, while if $n \geqslant g(d)$ then $H_{n,k}$ has maximal index. No graph other than $G_{n,k}$ or $H_{n,k}$ has maximal index for any value of n. In Section 4 we derive some bounds for the index of a graph in $\mathscr{H}(n, n+k)$.

2. SOME PRELIMINARY RESULTS

As in [1], let $\mathscr{S}(n, e)$ denote the set of all adjacency matrices of graphs with n vertices and e edges, and let $\mathscr{S}^*(n, e)$ be the subset of $\mathscr{S}(n, e)$ consisting of those matrices $A = (a_{ij})$ satisfying the condition

$$\text{if} \quad i < j \text{ and } a_{ij} = 1 \quad \text{then} \quad a_{hk} = 1 \quad \text{whenever } h < k \leqslant j \text{ and } h \leqslant i.$$

Following [9], we refer to a matrix in $\mathscr{S}^*(n, e)$ as a *stepwise* matrix. Brualdi and Solheid [2] show that a graph in $\mathscr{H}(n, e)$ with maximal index has an adjacency matrix $A = (a_{ij}) \in \mathscr{S}^*(n, e)$; it follows that $a_{12} = \cdots = a_{1n} = 1$. From the theory of irreducible nonnegative matrices [7] we know that there exists a unique positive unit vector $\mathbf{x}$ such that $A\mathbf{x} = \rho\mathbf{x}$, where ρ is the spectral radius of A. We shall refer to this vector $\mathbf{x}$ as the *principal eigenvector* of A. It is easily seen that if $\mathbf{x} = (x_1, \ldots, x_n)^T$ then $x_1 \geqslant x_2 \geqslant \cdots \geqslant x_n$ [9, Lemma 1].

Our standing assumption will be that $e = n + k$ where

$$k = \binom{d-1}{2} - 1 \qquad (*)$$

for some $d \leqslant n$. We may assume in fact that $4 < d < n$, because the cases

$d=2$, 3, and 4 have been dealt with in [2], and the case $d=n$ is trivial. (When $d=2$, $\binom{d-1}{2}$ is to be interpreted as zero, so that $e=n-1$.) Under the assumption $(*)$, the graph $G_{n,k}$ discussed in the introduction has a stepwise adjacency matrix $B=(b_{ij})$ given by

$$b_{1j}=1\ (2\leqslant j\leqslant n),\quad b_{ij}=1\ (2\leqslant i<j\leqslant d),\quad b_{ij}=0\ (i\geqslant 2,\ j>d).$$

Write $\gamma=\rho(G_{n,k})$, and let $\mathbf{y}=(y_1,\dots,y_n)^T$ be the principal eigenvector of B. Note that $y_2=\cdots=y_d$ and $y_{d+1}=\cdots=y_n$. The following equations hold:

$$\begin{aligned}(\gamma+1)y_1&=y_1+(d-1)y_2+(n-d)y_n,\\(\gamma+1)y_2&=y_1+(d-1)y_2,\\\gamma y_n&=y_1.\end{aligned}\tag{1}$$

If $k<n-3$, the graph $H_{n,k}$ has a stepwise adjacency matrix $C=(c_{ij})$ satisfying

$$\begin{aligned}&c_{1j}=1\quad(2\leqslant j\leqslant n),&&c_{2j}=1\quad(3\leqslant j\leqslant k+3),\\&c_{2j}=0\quad(j>k+3),&&c_{ij}=0\quad(3\leqslant i<j).\end{aligned}$$

Write $\chi=\rho(H_{n,k})$, and let $\mathbf{z}=(z_1,\dots,z_n)^T$ be the principal eigenvector of C. Then $z_3=\cdots=z_{k+3}$ and $z_{k+4}=\cdots=z_n$, and we have

$$\begin{aligned}(\chi+1)z_1&=z_1+z_2+(k+1)z_3+(n-k-3)z_n,\\(\chi+1)z_2&=z_1+z_2+(k+1)z_3,\\\chi z_3&=z_1+z_2,\\\chi z_n&=z_1.\end{aligned}\tag{2}$$

LEMMA 1. *Let*

$$d>4\quad\textit{and}\quad k=\binom{d-1}{2}-1<n-3.$$

Then one of the following holds:

(i) $\rho(H_{n,k}) < \rho(G_{n,k}) < d + \dfrac{4}{d-4}$;

(ii) $\rho(H_{n,k}) = \rho(G_{n,k}) = d + \dfrac{4}{d-4}$;

(iii) $\rho(H_{n,k}) > \rho(G_{n,k}) > d + \dfrac{4}{d-4}$.

Proof. Write $\gamma = \rho(G_{n,k})$, $\chi = \rho(H_{n,k})$. We follow Rowlinson [9] in considering $\mathbf{y}^T(B-C)\mathbf{z} = (\gamma - \chi)\mathbf{y}^T\mathbf{z}$. The matrix $B-C$ has $2r$ nonzero entries above the principal diagonal, where

$$r = \binom{d-2}{2},$$

and $\mathbf{y}^T(B-C)\mathbf{z} = \alpha - \beta$, say, where α is the sum of r terms of the form $y_i z_j + y_j z_i$ with $3 \leqslant i < j \leqslant d$, and $\beta = y_2(z_{d+1} + \cdots + z_{k+3}) + z_2(y_{d+1} + \cdots + y_{k+3})$. Thus $\alpha = 2ry_2z_3$ and $\beta = r(y_2z_3 + y_nz_2)$, so that $(\gamma - \chi)\mathbf{y}^T\mathbf{z} = r(y_2z_3 - y_nz_2)$. Suppose that $\chi < \gamma$. Then, since $\mathbf{y}^T\mathbf{z} > 0$, we have $y_2/y_n > z_2/z_3$. It follows from (1) that

$$\frac{y_2}{y_n} = \frac{\gamma}{\gamma - (d-2)}, \tag{3}$$

and from (2) that

$$\frac{z_2}{z_3} = \frac{\chi + \binom{d-1}{2}}{\chi + 1}. \tag{4}$$

Therefore

$$\frac{d-2}{\gamma - (d-2)} > \frac{\binom{d-1}{2} - 1}{\chi + 1} > \frac{\binom{d-1}{2} - 1}{\gamma + 1},$$

which leads to

$$\gamma < d + \frac{4}{d-4},$$

so that (i) holds. The assumptions $\chi = \gamma$, $\chi > \gamma$ similarly yield (ii), (iii) respectively. ∎

We can determine which of these three possibilities holds, for given n and d, by comparing $\rho(G_{n,k})$ with $d + 4/(d-4)$. This is done in Lemma 2, which involves the function g defined by

$$g(d) = \tfrac{1}{2}d(d+5) + 7 + \frac{32}{d-4} + \frac{16}{(d-4)^2} \qquad (d > 4). \tag{5}$$

LEMMA 2. *Let*

$$4 < d < n \quad \text{and} \quad k = \binom{d-1}{2} - 1.$$

Then

$$\rho(G_{n,k}) \lesseqqgtr d + \frac{4}{d-4} \quad \text{according as} \quad n \lesseqqgtr g(d).$$

Proof. From (1), $\gamma = \rho(G_{n,k})$ is the largest eigenvalue of the matrix

$$\begin{bmatrix} 0 & d-1 & n-d \\ 1 & d-2 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

and is therefore the largest zero of

$$f(t) = t^3 - (d-2)t^2 - (n-1)t + (d-2)(n-d).$$

It may be verified that

$$f\left(d + \frac{4}{d-4}\right) = \frac{2(d-2)}{d-4}[g(d) - n],$$

so that

$$\gamma > d + \frac{4}{d-4} \qquad \text{if} \quad n > g(d).$$

The results for $n \leqslant g(d)$ also follow if we verify that we then have $f(t) \geqslant 0$ whenever $t \geqslant d + 4/(d-4)$. For this it is enough to note that

$$f'\left(d + \frac{4}{d-4}\right) = d^2 + 4d + 17 + \frac{80}{d-4} + \frac{48}{(d-4)^2} - n > 0,$$

while $f''(t) = 6t - 2(d-2) > 0$ for all $t \geqslant d + 4/(d-4)$. ■

3. THE MAIN RESULT

THEOREM. *Let*

$$4 < d < n \quad \textit{and} \quad k = \binom{d-1}{2} - 1,$$

and let G be a graph of maximal index in $\mathscr{H}(n, n+k)$. *Then*

(i) $G = G_{n,k}$ *if* $n < g(d)$,
(ii) $G = G_{n,k}$ *or* $H_{n,k}$, *and* $\rho(G_{n,k}) = \rho(H_{n,k})$, *if* $n = g(d)$,
(iii) $G = H_{n,k}$ *if* $n > g(d)$,

where $g(d)$ *is defined by* (5).

Proof. Note first that if $n \geqslant g(d)$ then certainly $k < n-3$, so $H_{n,k}$ is defined and Lemma 1 may be applied. By virtue of the result of Brualdi and Solheid mentioned earlier, we know that G has a stepwise adjacency matrix A. Write $\rho = \rho(G)$, and let $\mathbf{x} = (x_1, \dots, x_n)^T$ be the principal eigenvector of A. Recall that $x_1 \geqslant x_2 \geqslant \cdots \geqslant x_n > 0$. As in Section 2, let $G_{n,k}$ and $H_{n,k}$ have stepwise adjacency matrices B, C respectively, with corresponding principal eigenvectors $\mathbf{y}, \mathbf{z}$, and write $\gamma = \rho(G_{n,k})$, $\chi = \rho(H_{n,k})$.

(i): Let $n < g(d)$ and suppose that $G \neq G_{n,k}$: we shall prove that $\rho(G) < \rho(G_{n,k})$. Suppose that the matrix $B - A$ has $2r$ nonzero entries above the principal diagonal. Then $(\gamma - \rho)\mathbf{x}^T\mathbf{y} = \mathbf{x}^T(B-A)\mathbf{y} = \alpha - \beta$, where α is the sum of r terms $x_i y_j + x_j y_i$ for which $3 \leqslant i < j \leqslant d$, and β is the sum of r such terms for which $2 \leqslant i < j$ and $j \geqslant d+1$. Thus $\alpha \geqslant r(x_{d-1}y_2 + x_d y_2) \geqslant 2rx_d y_2$, and $\beta \leqslant r(x_2 y_n + x_{d+1}y_2) \leqslant r(x_2 y_n + x_d y_2)$, so that $(\gamma - \rho)\mathbf{x}^T\mathbf{y} \geqslant r(x_d y_2 - x_2 y_n)$.

Suppose, by way of contradiction, that $\gamma \leqslant \rho$: then

$$\frac{x_2}{x_d} \geqslant \frac{y_2}{y_n}. \tag{6}$$

Let h be maximal such that $a_{hd} = 1$, and let m be maximal such that $a_{2m} = 1$. (See Figure 1.) Since $A \neq B$, we have $2 \leqslant h \leqslant d-2$ and $d+1 \leqslant m \leqslant n$. Let $2u$ be the number of entries a_{ij} with $h+1 \leqslant i \leqslant d$, $h+1 \leqslant j \leqslant d$ which are equal to 1. Then

$$(\rho+1)x_2 = \sum_{i=1}^{h} x_i + \sum_{i=h+1}^{m} x_i = \rho x_d + \frac{1}{\rho} \sum_{i=h+1}^{m} \rho x_i$$

$$\leqslant \rho x_d + \frac{1}{\rho}\left\{(m-h)\sum_{i=1}^{h} x_i + 2u x_{h+1}\right\}$$

$$\leqslant (\rho+m-h)x_d + \frac{2u}{\rho} x_h \tag{7}$$

$$\leqslant (\rho+m-h)x_d + \frac{2u}{\rho}\cdot\frac{1}{h}\sum_{i=1}^{h} x_i$$

$$= \left(\rho+m-h+\frac{2u}{h}\right)x_d$$

$$\leqslant [\rho+m-h+(h-2)(d-h)+u]x_d. \tag{8}$$

Now

$$m-h+(h-2)(d-h)+u \leqslant \binom{d-1}{2},$$

because the expression on the left is less than or equal to the number of entries a_{ij} with $2 = i < j$ or $3 \leqslant i < j \leqslant d$ which are equal to 1. Thus

$$(\rho+1)x_2 \leqslant \left[\rho + \binom{d-1}{2}\right]x_d,$$

$$
\begin{array}{c|cccccccccccccccccc}
 & & & & (h) & & & & (c) & & & & (d) & & & (m) & & & (n) \\
 & 0 & 1 & 1 \cdots & 1 & 1 & 1 & \cdots & 1 & 1 & & \cdots & 1 & 1 & \cdots & 1 & 1 & \cdots & 1 \\
 & & 0 & 1 \cdots & 1 & 1 & 1 & \cdots & 1 & 1 & & \cdots & 1 & 1 & \cdots & 1 & 0 & \cdots & 0 \\
 & & & \ddots & \vdots & \vdots & \vdots & & \vdots & \vdots & & & \vdots & * & & & & & \\
(h) & & & & 0 & 1 & 1 & \cdots & 1 & 1 & & \cdots & 1 & & & & & & \\
 & & & & & 0 & 1 & \cdots & 1 & 1 & & & 0 & & & & & & \\
 & & & & & 1 & 0 & \cdots & 1 & 1 & & & 0 & & & & & & \\
 & & & & & \vdots & & \ddots & \vdots & \vdots & * & & \vdots & & & & & & \\
(c) & & & & & 1 & 1 & \cdots & 0 & 1 & & & 0 & & & & & & \\
 & & & & & 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & & & & & & \\
 & & & & & & & & & 0 & 0 & \cdots & 0 & & & & & & \\
 & & & & & & & * & & \vdots & & \ddots & \vdots & & & & & & \\
(d) & & & & & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & & & & & &
\end{array}
$$

FIG. 1. Part of the matrix A.

and it follows from (3) and (6) that

$$\frac{\gamma}{\gamma-(d-2)} \leqslant \frac{\rho+\binom{d-1}{2}}{\rho+1}.$$

This leads to $\gamma \geqslant d+4/(d-4)$, but Lemma 2 then gives the contradiction $n \geqslant g(d)$. Thus $\rho < \gamma$, as asserted.

(ii): Let $n = g(d)$; then

$$\gamma = \chi = d + \frac{4}{d-4}$$

by Lemma 1. Suppose that G is not equal to either $G_{n,k}$ or $H_{n,k}$. If we assume that $\gamma \leqslant \rho$, then the argument of (i) leads to the conclusion that $\gamma > d+4/(d-4)$, unless equality holds throughout. But we need $u = 0$ for equality in (7), because $(\rho+1)x_h \geqslant (\rho+1)x_{h+1} + x_d$, so that $x_{h+1} < x_h$; and for equality in (8) we must have $h = 2$. However, if $u = 0$ and $h = 2$ then $A = C$, a further contradiction. Thus $\rho < \gamma$.

(iii): Let $n > g(d)$, and suppose that $G \neq H_{n,k}$. Define h and m as in the proof of (i): this time we have $2 \leqslant h \leqslant d-1$ and $d \leqslant m < k+3 < n$. Let c be maximal such that $a_{c,c+1} = 1$. (See Figure 1.) Since $A \neq C$, we have

$3 \leqslant c \leqslant d-1$. For $3 \leqslant i \leqslant c$, let $m(i)$ be maximal such that $a_{i,m(i)} = 1$. Then $\Sigma_{i=3}^{c}[m(i)-i] = r$, where r is the number of entries a_{ij} with $3 \leqslant i < j$ which are equal to 1. (We also have $r = k+3-m$.) Let v be the number of entries a_{ij} with $h+1 \leqslant i < j \leqslant d$ which are equal to 0; then v is also the number of entries a_{ij} with $2 \leqslant i \leqslant h$, $d+1 \leqslant j \leqslant m$ which are equal to 1. Consider $(\chi - \rho)\mathbf{x}^T\mathbf{z} = \mathbf{x}^T(C - A)\mathbf{z} = \alpha - \beta$, where $\alpha = x_2(z_{m+1} + \cdots + z_{k+3}) + z_2(x_{m+1} + \cdots + x_{k+3})$, and β is the sum of r terms $x_i z_j + x_j z_i$ for which $3 \leqslant i \leqslant c$, $i+1 \leqslant j \leqslant m(i)$. Since $x_{m+1} = \cdots = x_n$ we have $\alpha = r(x_2 z_3 + z_2 x_n)$. Also, $\beta \leqslant r x_2 z_3 + z_3 \Sigma_{i=3}^{c} \Sigma_{j=i+1}^{m(i)} x_j = r(x_2 + q) z_3$, where $q = (1/r)\Sigma_{i=3}^{c}\Sigma_{j=i+1}^{m(i)} x_j$. Therefore $(\chi - \rho)\mathbf{x}^T\mathbf{z} > r(x_n z_2 - q z_3)$. Suppose, by way of contradiction, that $\rho \geqslant \chi$: then

$$\frac{q}{x_n} \geqslant \frac{z_2}{z_3}. \tag{9}$$

We will show that

$$\frac{q}{x_n} \leqslant \frac{\rho}{\rho - (d-2)}. \tag{10}$$

To this end, write $q = q_1 + q_2$, where

$$q_1 = \frac{1}{r}\sum_{i=3}^{h}\sum_{j=i+1}^{m(i)} x_j, \qquad q_2 = \frac{1}{r}\sum_{i=h+1}^{c}\sum_{j=i+1}^{m(i)} x_j.$$

(Put $q_1 = 0$ if $h = 2$, and $q_2 = 0$ if $h = c$.)

For each $i \in \{3, \ldots, h\}$ we have $m(i) \geqslant d$, and therefore, since $x_2 \geqslant \cdots \geqslant x_m$,

$$\frac{\Sigma_{j=i+1}^{m(i)} x_j}{m(i) - i} \leqslant \frac{\Sigma_{j=2}^{d} x_j}{d-1} = a_1, \qquad \text{say.}$$

Thus

$$q_1 \leqslant \frac{a_1}{r}\sum_{i=3}^{h}[m(i) - i].$$

Now

$$(\rho+1)a_1=\frac{1}{d-1}\sum_{j=2}^{d}(\rho+1)x_j$$

$$=\frac{1}{d-1}\left\{(d-1)\sum_{i=1}^{d}x_i+(v \text{ terms } x_s)-(2v \text{ terms } x_t)\right\},$$

where each $s \geqslant d+1$ and each $t \leqslant d$. Hence

$$(\rho+1)a_1 \leqslant \frac{1}{d-1}\{(d-1)[x_1+(d-1)a_1]-vx_d\}$$

$$\leqslant x_1+(d-1)a_1.$$

Thus $[\rho-(d-2)]a_1 \leqslant x_1$, so that

$$[\rho-(d-2)]q_1 \leqslant \frac{x_1}{r}\sum_{i=3}^{h}[m(i)-i]. \tag{11}$$

Turning now to q_2, we note that

$$x_{h+1} < \frac{\sum_{i=1}^{d}x_i}{\rho+1}=a_2, \qquad \text{say.}$$

It follows that if $i \geqslant h+1$, then for each $j \in \{i+1,\dots,m(i)\}$ we have $x_j < a_2$, so that

$$q_2 \leqslant \frac{a_2}{r}\sum_{i=h+1}^{c}[m(i)-i].$$

From the above, we have $(\rho+1)\sum_{i=2}^{d}x_i \leqslant (d-1)\sum_{i=1}^{d}x_i$, and it follows that

$$(\rho+1)a_2 \leqslant x_1+(d-1)a_2.$$

Thus $[\rho-(d-2)]a_2 \leqslant x_1$, so that

$$[\rho-(d-2)]q_2 \leqslant \frac{x_1}{r} \sum_{i=h+1}^{c} [m(i)-i]. \tag{12}$$

From (11) and (12), $[\rho-(d-2)]q \leqslant x_1 = \rho x_n$, and (10) is established. From (4), (9), and (10) we obtain

$$\frac{\chi+\binom{d-1}{2}}{\chi+1} \leqslant \frac{\rho}{\rho-(d-2)},$$

and this leads to $\chi \leqslant d+4/(d-4)$. Lemmas 1 and 2 then give the contradiction $n \leqslant g(d)$. Thus $\rho < \chi$. ■

COROLLARY 1. *When e is of the form*

$$e = n-1+\binom{d-1}{2} \qquad \textit{for some} \quad d \in \{2,\dots,n\},$$

$\mathscr{H}(n,e)$ has a unique graph of maximal index, except in the three cases $n=60$, $e=69$; $n=68$, $e=88$; $n=80$, $e=85$.

Proof. When $d=2$, 3, or 4 the result is known from [2], and when $d=n$ it is trivial. When $d \in \{5,\dots,n-1\}$, it follows from the theorem that there is a unique graph of maximal index unless $n=g(d)$, and for $g(d)$ to be an integer we need $d=5$, 6, or 8. ■

COROLLARY 2. *Let $e=n+k$, where*

$$k = \binom{d-1}{2}-1 \qquad \textit{for some} \quad d \in \{2,\dots,n\}.$$

If (i) $n<60$ *or* (ii) $e \geqslant 2n-47$, *then $G_{n,k}$ is the unique graph in $\mathscr{H}(n,e)$ of maximal index.*

Proof. When $d=2$, 3, or 4, the result is known from [2], without the need for either of the conditions (i) and (ii); and when $d=n$ it is trivial. When $d \in \{5,\dots,n-1\}$ we have to show that if (i) or (ii) applies then

$n > g(d)$. It is easily checked that the minimum value of $g(d)$ for integers $d \geqslant 5$ is $g(6) = 60$, so that (i) is immediate. For (ii), note that if $e \geqslant 2n - 47$ then $n \leqslant \frac{1}{2}d(d-3) + 47$, so

$$g(d) - n \geqslant 4(d-10) + \frac{32}{d-4} + \frac{16}{(d-4)^2} > 0 \qquad \text{for all} \quad d \geqslant 5. \qquad \blacksquare$$

REMARK. The constant 47 in Corollary 2(ii) cannot be improved, because when $n = 62$ and $e = 76$ we have $e = 2n - 48$ and $H_{62,14}$ has maximal index. The coefficient 2 is also best possible, in the sense that if $\lambda < 2$ then there exist values of n and e of the required form, with $e > \lambda n$ and such that $H_{n,k}$ has maximal index in $\mathscr{H}(n, e)$. This is because if $n = g(d)$ then

$$\frac{e}{n} = 1 + \frac{\frac{1}{2}d(d-3)}{g(d)} \to 2 \qquad \text{as} \quad d \to \infty.$$

We can obtain a more precise expression of the relation between e and n at the "transition state" by inverting the condition $n = g(d)$. We obtain

$$d = \sqrt{2n} - \frac{5}{2} - \frac{31}{8\sqrt{2n}} + O\left(\frac{1}{n}\right),$$

so that

$$e = 2n - 4\sqrt{2n} + 3 + O\left(\frac{1}{\sqrt{n}}\right),$$

as $n \to \infty$ with $n = g(d)$.

4. SOME BOUNDS FOR THE INDEX

PROPOSITION 1. *Let $e = n + k$, where*

$$k = \binom{d-1}{2} - 1 \qquad \textit{for some} \quad d \in \{5, \ldots, n-1\},$$

and write

$$b_1(n,d) = \sqrt{n + \tfrac{1}{2}d^2 - \tfrac{5}{2}d + 1}\,, \qquad b_2(n,d) = \sqrt{n + d^2 - 3d + 1}\,.$$

Then

(i) $\max(d-1, b_1(n,d)) \leqslant \rho(G_{n,k}) \leqslant \min\left(d + \dfrac{4}{d-4}, b_2(n,d)\right)$ *if* $n \leqslant g(d)$,

(ii) $\max\left(d + \dfrac{4}{d-4}\right), \sqrt{n-1}\,) \leqslant \rho(G_{n,k}) \leqslant \rho(H_{n,k}) \leqslant b_1(n,d)$ *if* $n \geqslant g(d)$.

Proof. For simplicity we write $b_1 = b_1(n,d)$, $b_2 = b_2(n,d)$, and we denote $\rho(G_{n\cdot k}), \rho(H_{n,k})$ by γ, χ as before. The only inequalities requiring comment are

(i) $b_1 \leqslant \gamma \leqslant b_2$ when $n \leqslant g(d)$,
(ii) $\chi \leqslant b_1$ when $n \geqslant g(d)$.

For (i), recall that γ is the largest zero of

$$f(t) = t^3 - (d-2)t^2 - (n-1)t + (d-2)(n-d). \tag{13}$$

Suppose that $n \leqslant g(d)$. This implies that $b_1 \leqslant d + 4/(d-4)$, and it is easily verified that

$$f(b_1) = \tfrac{1}{2}(d-1)(d-4)\left[b_1 - \left(d + \frac{4}{d-4}\right)\right] \leqslant 0.$$

Thus $\gamma \geqslant b_1$ [with equality when $n = g(d)$]. To see that $\gamma \leqslant b_2$, note that

$$b_2 = \sqrt{(d-1)^2 + (n-d)} \geqslant d-1,$$

so $f(b_2) = (d-1)(d-2)[b_2 - (d-1)] \geqslant 0$. It may be checked that $f'(b_2) > 0$ and $f''(t) \geqslant 0$ for all $t \geqslant b_2$, so that $f(t) \geqslant 0$ for all $t \geqslant b_2$. It follows that $\gamma \leqslant b_2$.

For (ii), note that χ is the largest eigenvalue of the matrix

$$\begin{bmatrix} 0 & 1 & k+1 & n-k-3 \\ 1 & 0 & k+1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

Thus χ is the largest zero of $h(t)$, where

$$h(t) = t^4 - (n+k)t^2 - 2(k+1)t + (k+1)(n-k-3). \qquad (14)$$

Suppose that $n \geqslant g(d)$: this gives $b_1 \geqslant d + 4/(d-4)$. Routine calculations show that

$$h(b_1) = \tfrac{1}{2}(d-1)(d-4)\left[b_1 - \left(d + \frac{4}{d-4}\right)\right](b_1 + d - 2) \geqslant 0,$$

and that $h'(b_1) > 0$, $h''(t) > 0$ for all $t \geqslant b_1$. Thus $\chi \leqslant b_1$ [with equality when $n = g(d)$]. ∎

Note that if

$$\binom{d-1}{2} + 3 \leqslant n \leqslant g(d)$$

then $H_{n,k}$ is defined, and we may replace (i) by

$$\text{(i}'\text{)} \qquad \max(d-1, b_1(n,d)) \leqslant \rho(H_{n,k}) \leqslant \rho(G_{n,k}) \leqslant \min\left(d + \frac{4}{d-4}, b_2(n,d)\right),$$

because we then have $h(b_1) \leqslant 0$, and therefore $\chi \geqslant b_1$.

From Proposition 1 and the theorem we obtain

Proposition 2. *Let* $e = n + k$, *where*

$$k = \binom{d-1}{2} - 1 \qquad \textit{for some} \quad d \in \{5, \ldots, n-1\},$$

and let G be any graph in $\mathscr{H}(n,e)$. *Then*

$$\rho(G) \leqslant \begin{cases} \min\left(d + \dfrac{4}{d-4}, b_2(n,d)\right) & \textit{if} \quad n \leqslant g(d), \\ b_1(n,d) & \textit{if} \quad n > g(d). \end{cases}$$

CONCLUDING REMARKS.

1. Since $b_1(n,d) < b_2(n,d) = \sqrt{2e-n+1}$, we deduce that $\rho(G) \leqslant \sqrt{2e-n+1}$ for all graphs in $\mathscr{H}(n,e)$, if e is of the given form. This bound has been shown to be valid for arbitrary e and n by Yuan [10], using a quite different method. The bound in Proposition 2 represents an improvement on $\sqrt{2e-n+1}$ whenever

$$n > 3d + 7 + \frac{32}{d-4} + \frac{16}{(d-4)^2},$$

because $d + 4/(d-4) < b_2(n,d)$ for such n.

2. When d (> 4) is fixed and

$$k = \binom{d-1}{2} - 1,$$

the difference between the indices of $G_{n,k}$ and $H_{n,k}$ is surprisingly small for large values of n. Routine calculations using (13) and (14) lead to

$$\rho(G_{n,k}) = \sqrt{n} - \frac{1}{2\sqrt{n}} + \binom{d-1}{2} \cdot \frac{1}{n} + \tfrac{1}{8}(4d^3 - 20d^2 + 32d - 17) \cdot \frac{1}{n^{3/2}} + O\left(\frac{1}{n^2}\right),$$

and

$$\rho(H_{n,k}) = \sqrt{n} - \frac{1}{2\sqrt{n}} + \binom{d-1}{2} \cdot \frac{1}{n} + \tfrac{1}{8}(d^4 - 6d^3 + 15d^2 - 18d + 7) \cdot \frac{1}{n^{3/2}} + O\left(\frac{1}{n^2}\right).$$

Thus, for fixed $d > 4$,

$$\rho(H_{n,k}) - \rho(G_{n,k}) \sim \tfrac{1}{8}(d-1)(d-2)(d-3)(d-4) \cdot \frac{1}{n^{3/2}} \qquad \text{as} \quad n \to \infty.$$

3. When

$$k = \binom{d-1}{2} - 1$$

for a fixed $d > 4$, and n is sufficiently large, we have $\rho(G) \leqslant \sqrt{n}$ for all G in $\mathscr{H}(n, n+k)$. How large must n be? It is straightforward to deduce from (14) that $\rho(H_{n,k}) \leqslant \sqrt{n}$ if and only if $n \geqslant N(d)$, where

$$N(d) = \left[\tfrac{1}{2}(d-1)(d-2) + \sqrt{\tfrac{1}{2}(d-1)(d-2)(d^2-3d+4)}\,\right]^2.$$

Thus $\rho(G) \leqslant \sqrt{n}$ whenever $n \geqslant N(d)$, and therefore whenever $n \geqslant cd^4$, where $c = (3+2\sqrt{2})/4 \approx 1.457$.

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