

# On the Maximal Index of Graphs with a Prescribed Number of Edges

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## ABSTRACT

Among the graphs with a prescribed number of edges, those with maximal index are determined. The result confirms a conjecture of Brualdi and Hoffman.

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## 1. INTRODUCTION

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  $G$ . For  $e > 0$ , let  $\mathcal{S}(e)$  denote the set of all graphs with precisely  $e$  edges. The problem of finding the graphs in  $\mathcal{S}(e)$  with maximal index was posed by Brualdi and Hoffman in 1976 (cf. [1, p. 438]), and their results appeared some ten years later [2]. They showed that if  $f(e)$  denotes the maximal index of a graph with  $e$  edges, and if  $d > 1$ , then

$$f\left(\binom{d}{2}\right) = d - 1$$

with equality precisely when the only nontrivial component of the graph is  $K_d$  (the complete graph on  $d$  vertices). They conjectured that when

$$\binom{d}{2} < e < \binom{d+1}{2}$$

the maximal index is attained precisely when the only nontrivial component

is the graph  $G_e$  obtained from  $K_d$  by adding one new vertex of degree

$$t = e - \binom{d}{2}.$$

By applying perturbation-theoretic methods to adjacency matrices, Friedland [3] proved that there exists  $K(t) > 0$  such that the conjecture is true for  $d \geq K(t)$ . He also proved that the conjecture is true for  $t = d - 1$ . Subsequently, Stanley [6] proved that  $f(e) \leq \frac{1}{2}(-1 + \sqrt{1 + 8e})$ , with equality precisely when  $e = \binom{d}{2}$ . Friedland [4] refined Stanley's inequality and thereby proved the conjecture for  $t = 1$ ,  $t = d - 3$ , and  $t = d - 2$ . Here we prove that the conjecture is true in general.

## 2. SOME PRELIMINARY RESULTS

As in [2],  $\mathcal{S}(n, e)$  denotes the set of adjacency matrices of graphs with  $n$  vertices and  $e$  edges, and  $\mathcal{S}^*(n, e)$  denotes 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  $h \leq i$ .

In view of the distribution of nonzero entries in a matrix belonging to  $\mathcal{S}^*(n, e)$ , we call such a matrix a *stepwise* matrix. Note that a nonzero stepwise matrix  $A$  is the adjacency matrix of a graph with a unique nontrivial component. It follows from the theory of nonnegative matrices [5, Chapter XIII] that if  $\rho(A)$  is the largest eigenvalue of the stepwise matrix  $A$ , then there exists a unique nonnegative unit vector  $\mathbf{x} = (x_1, \dots, x_n)^T$  such that  $A\mathbf{x} = \rho(A)\mathbf{x}$ ; moreover,  $x_i = 0$  if and only if vertex  $i$  is isolated.

**LEMMA 1.** *Let  $A \in \mathcal{S}^*(n, e)$ ,  $e > 0$ . If  $(x_1, \dots, x_n)^T$  is a nonnegative eigenvector corresponding to  $\rho(A)$ , then  $x_1 \geq \dots \geq x_n$ .*

*Proof.* We give a detailed proof of this straightforward result in order to establish notation and equations for subsequent use. Note that there exists  $m \leq n$  such that  $x_i > 0$  for  $1 \leq i \leq m$  and  $x_i = 0$  for  $m < i \leq n$ . We suppose that  $e < \binom{n}{2}$ , for otherwise  $x_1 = \dots = x_n$ . Let  $A = (a_{ij})$ , and let  $c$  be least

such that  $a_{c,c+1} = 0$ . Writing  $\rho = \rho(A)$ , we have

$$x_1 + \dots + x_r = \begin{cases} (\rho + 1)x_i & \text{if } 1 \leq i \leq c, \\ \rho x_i & \text{if } c+1 \leq i \leq m, \end{cases} \quad (1)$$

where  $m \geq r_1 \geq r_2 \geq \dots \geq r_c = c > r_{c+1} \geq r_{c+2} \geq \dots \geq r_m > 0$ . Hence  $x_1 \geq x_2 \geq \dots \geq x_c$  and  $x_{c+1} \geq x_{c+2} \geq \dots \geq x_m$ . Moreover,  $\rho(x_c - x_{c+1}) = (x_1 + \dots + x_{c-1}) - (x_1 + \dots + x_{r_{c+1}})$ , which is nonnegative because  $r_{c+1} \leq c - 1$ . Since  $\rho > 0$ , we have  $x_c \geq x_{c+1}$ . ■

Let  $\mathcal{S}^{**}(n, e)$  be the subset of  $\mathcal{S}^*(n, e)$  consisting of those matrices  $A = (a_{ij})$  satisfying

(\*\*\*) if

- (i)  $h < p < q < k$ , and
- (ii)  $a_{hk} = 1$ ,  $a_{hj} = 0$  whenever  $j > k$ ,  $a_{ik} = 0$  whenever  $i > h$ , and
- (iii)  $a_{pq} = 0$ ,  $a_{pj} = 1$  whenever  $p < j < q$ ,  $a_{iq} = 1$  whenever  $i < p$ , then  $p + q \leq h + k + 1$ .

Figure 1 shows a matrix in  $\mathcal{S}^{**}(32, 224)$ : for this matrix, the values of  $(h, k)$  ( $h < k$ ) which satisfy condition (ii) are  $(3, 29)$ ,  $(10, 25)$ ,  $(11, 21)$ , and  $(13, 16)$ ; the values of  $(p, q)$  ( $p < q$ ) which satisfy condition (iii) are  $(4, 26)$ ,  $(11, 22)$ ,  $(12, 17)$ , and  $(14, 15)$ .

Let  $f(n, e)$ ,  $f^*(n, e)$ ,  $f^{**}(n, e)$  denote the maximum value of  $\rho(A)$  attained by a matrix in  $\mathcal{S}(n, e)$ ,  $\mathcal{S}^*(n, e)$ ,  $\mathcal{S}^{**}(n, e)$  respectively. Brualdi and Hoffman [2] proved that  $f(n, e) = f^*(n, e)$ ; moreover if  $A \in \mathcal{S}(n, e)$  and  $\rho(A) = f^*(n, e)$ , then there exists a permutation matrix  $P$  such that  $P^{-1}AP \in \mathcal{S}^*(n, e)$ . The next result shows that these statements remain true when  $\mathcal{S}^*(n, e)$  is replaced by  $\mathcal{S}^{**}(n, e)$  and  $f^*(n, e)$  is replaced by  $f^{**}(n, e)$ .

**LEMMA 2.** *If  $A \in \mathcal{S}^*(n, e)$  and  $A \notin \mathcal{S}^{**}(n, e)$ , then there exists  $A' \in \mathcal{S}^*(n, e)$  such that  $\rho(A) < \rho(A')$ .*

*Proof.* In respect of the matrix  $A = (a_{ij})$ , there exist indices  $h, p, q, k$  satisfying conditions (i), (ii), and (iii) of property (\*\*\*) such that  $p + q \geq h + k + 2$ . Since  $e < \binom{n}{2}$ , there exists a least  $c$  such that  $a_{c,c+1} = 0$ . Note that  $h < p \leq c < q < k$  and  $e > 0$ . Let  $\rho = \rho(A)$ , and let  $x = (x_1, \dots, x_n)^T$  be the nonnegative unit eigenvector of  $A$  corresponding to  $\rho$ . In the notation of Lemma 1, we have  $r_h = k$ ,  $r_p = q - 1$ ,  $r_q = p - 1$ , and  $r_k = h$ .

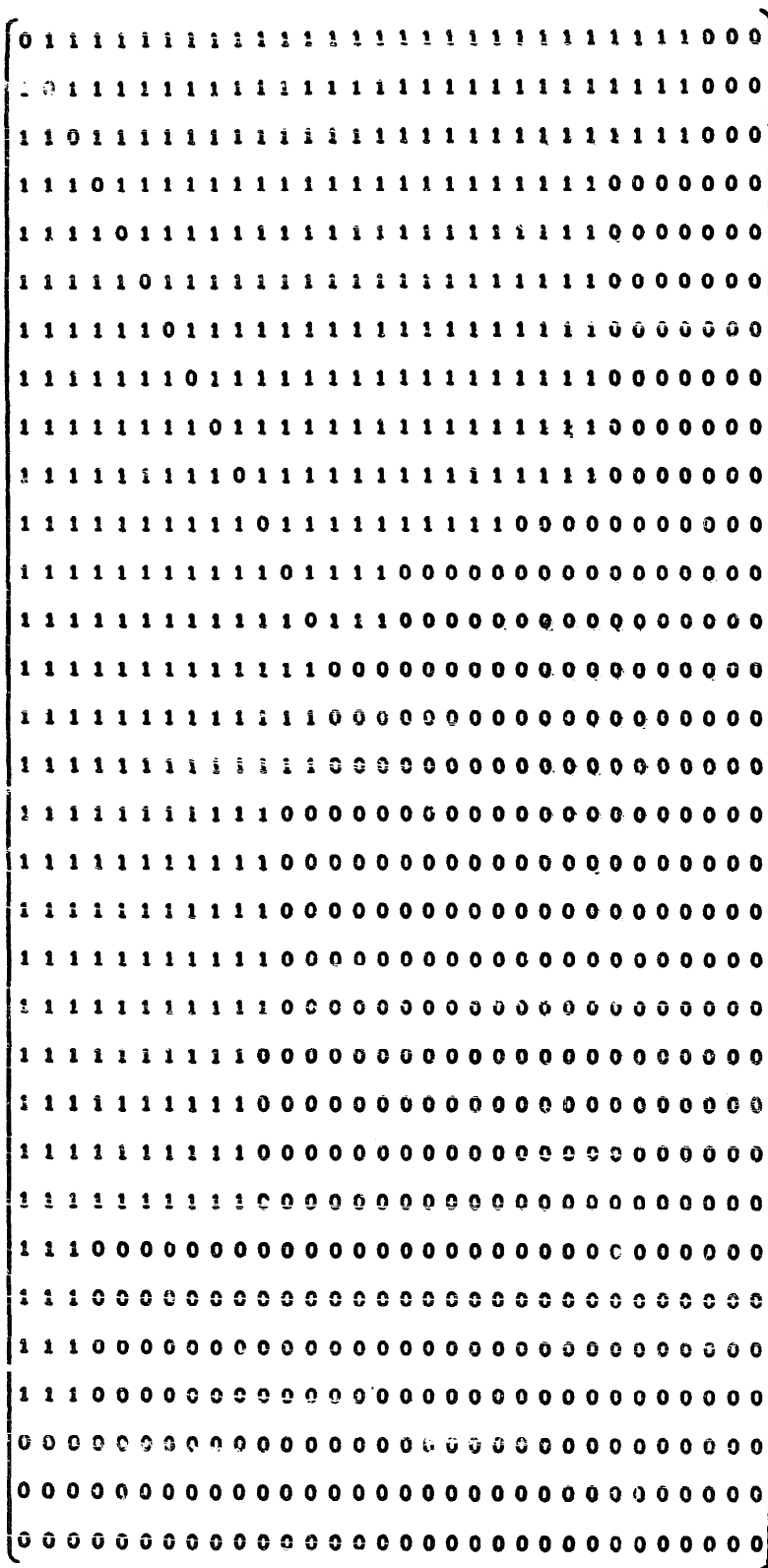


FIG. 1. A matrix in  $\mathcal{S}^{**}(32, 224)$ .

Let  $A'$  be the matrix obtained from  $A$  by interchanging the  $(h, k)$  and  $(p, q)$  entries and interchanging the  $(k, h)$  and  $(q, p)$  entries. Then  $A' \in \mathcal{S}^*(n, e)$ . Since  $\rho(A') = \sup\{z^T A' z : z^T z = 1\}$  and  $x^T A x = \rho$ , it suffices to prove that  $x^T A' x > x^T A x$ . Now  $x^T (A' - A)x = 2(x_p x_q - x_h x_k)$ , and from the equations (1) we have

$$\begin{aligned} & \rho^2(x_p x_q - x_h x_k) \\ &= [(x_1 + \cdots + x_{h-1}) + (x_h + \cdots + x_{q-1}) - x_p] \\ & \quad \times [(x_1 + \cdots + x_{h-1}) + (x_h + \cdots + x_{p-1})] \\ & \quad - [(x_1 + \cdots + x_{h-1}) + (x_{h+1} + \cdots + x_k)] [(x_1 + \cdots + x_{h-1}) + x_h] \\ &= (x_1 + \cdots + x_{h-1}) [(x_h + \cdots + x_{q-1}) - x_p \\ & \quad + (x_h + \cdots + x_{p-1}) - (x_h + \cdots + x_k)] \\ & \quad + [(x_h + \cdots + x_{q-1}) - x_p] (x_h + \cdots + x_{p-1}) - x_h (x_{h+1} + \cdots + x_k) \\ &= (x_1 + \cdots + x_{h-1}) [(x_h + \cdots + x_{q-1}) - x_p - (x_p + \cdots + x_k)] \\ & \quad + x_h [(x_{h+1} + \cdots + x_{p-1}) - (x_q + \cdots + x_k)] \\ & \quad + [(x_{h+1} + \cdots + x_{q-1}) - x_p] (x_{h+1} + \cdots + x_{p-1}) + x_h (x_h - x_p). \end{aligned}$$

We use Lemma 1 to show that each of these four summands is nonnegative, the last nonzero. First,  $(x_h + \cdots + x_{q-1}) - x_p - (x_p + \cdots + x_k) \geq (x_{h+1} + \cdots + x_{q-1}) - (x_p + \cdots + x_k)$ , which is nonnegative because  $x_{h+1} \geq x_p$  and  $(q-1) - h \geq k - (p-1)$ . Secondly,  $(x_{h+1} + \cdots + x_{p-1}) - (x_q + \cdots + x_k) \geq 0$  because  $x_{h+1} \geq x_q$  and  $(p-1) - h \geq k - (q-1)$ . Thirdly,  $(x_{h+1} + \cdots + x_{q-1}) - x_p \geq 0$  because  $h+1 \leq p \leq q-1$ ; and fourthly,  $x_h(x_h - x_p) = x_h(x_q + \cdots + x_k) / (\rho + 1)$ , which is positive because vertices  $1, 2, \dots, k$  lie in the nontrivial component of the graph with adjacency matrix  $A$ . ■

## 3. THE MAIN RESULT

**THEOREM.** *Let*

$$e = \binom{d}{2} + t, \quad \text{where } 0 < t < d,$$

and let  $G_e$  be the graph obtained from the complete graph  $K_d$  by adding one new vertex of degree  $t$ . If  $G$  is a graph with maximal index among the graphs with  $e$  edges, then  $G$  has a unique nontrivial component  $H$  and  $H = G_e$ .

*Proof.* Let  $A = (a_{ij}) \in \mathcal{S}^{**}(n, e)$ , and suppose that the graph  $G$  with adjacency matrix  $A$  does not satisfy the conclusions of the Theorem. Note that  $n \geq d + 1$ . By Lemma 2 it suffices to prove that  $\rho(A) < \rho(A')$ , where  $A'$  is an adjacency matrix of the graph  $G'$  obtained from  $G_e$  by adding  $n - (d + 1)$  isolated vertices. We suppose that the vertices of  $G'$  are labeled so that  $A' \in \mathcal{S}^{**}(n, e)$ , and we let  $\rho = \rho(A)$ ,  $\rho' = \rho(A')$ . Let  $\mathbf{x}, \mathbf{x}'$  be the unique nonnegative unit eigenvectors of  $A, A'$  corresponding to  $\rho, \rho'$  respectively, say  $\mathbf{x} = (x_1, \dots, x_n)^T$  and  $\mathbf{x}' = (x'_1, \dots, x'_n)^T$ . Note that  $x'_1 = \dots = x'_t$  and  $x'_{t+1} = \dots = x'_d$ . In respect of the matrix  $A'$  the equations (1) reduce to:

$$(\rho' + 1)x'_1 = tx'_1 + (d - t)x'_d + x'_{d+1}, \quad (1a)$$

$$(\rho' + 1)x'_d = tx'_1 + (d - t)x'_d, \quad (1b)$$

$$\rho'x'_{d+1} = tx'_1. \quad (1c)$$

On subtracting (1b) and (1c) from (1a), we obtain

$$x'_d + x'_{d+1} = x'_1 + x'_1 t(\rho' + 1)^{-1}. \quad (2)$$

Let  $c$  be minimal such that  $a_{c, c+1} = 0$ , and let  $v$  be maximal such that  $a_{v, d+1} \neq 0$ . In investigating the sign of  $\rho' - \rho$ , we distinguish two cases: (I)  $v \leq t$ , (II)  $v > t$ . In case (I), we have  $\mathbf{x}'^T(\rho' - \rho)\mathbf{x}' = \mathbf{x}'^T(A' - A)\mathbf{x}' = \alpha - \beta$ , where  $\alpha$  is the sum of (say)  $r$  terms  $x'_i x'_j + x'_i x'_j$  for which  $v + 1 \leq i \leq d$ ,  $c + 1 \leq j \leq d + 1$ , and  $i < j$ ; and  $\beta$  is the sum of  $r$  terms  $x'_i x'_j + x'_i x'_j$  for which  $1 \leq i \leq v$ ,  $d + 2 \leq j \leq n$ , and  $i < j$ . By Lemma 1, we have  $\alpha \geq r(x'_d + x'_{d+1})x'_{d+1}$ ; then by Equation (2),  $\alpha > rx'_1 x'_{d+1}$ . On the other hand, since  $x'_j = 0$  for  $j \geq d + 2$ , we have  $\beta \leq rx'_1 x'_{d+2}$ . Hence  $\rho' > \rho$  because  $\mathbf{x}'^T \mathbf{x}' > 0$  and  $\alpha - \beta > 0$ .

In case (II), again let  $2r$  be the number of entries equal to 1 in the matrix  $A' - A$ . We distinguish two subcases: (IIa)  $r \geq t$ , (IIb)  $r < t$ . We show next that in subcase (IIa) we have  $\rho \leq d - 1$ : since  $\rho' > d - 1$ , we again have  $\rho' > \rho$ . Let  $A''$  be the matrix obtained from  $A'$  by making the  $(d + 1)$ th column a zero column and the  $(d + 1)$ th row a zero row. Then  $\rho(A'') = d - 1$ , and the corresponding nonnegative unit eigenvector  $x'' = (x''_1, \dots, x''_n)^T$  has  $x''_1 = \dots = x''_d, x''_{d+1} = \dots = x''_n = 0$ . Now  $x^T x''(d - 1 - \rho) = x^T(A'' - A)x'' = \alpha - \beta$ , where  $\alpha$  is a sum of  $r$  terms  $x''_i x_j + x_i x''_j$  for which  $v + 1 \leq i \leq d - 1, c + 1 \leq j \leq d$ , and  $i < j$ ; and  $\beta$  is a sum of  $r + t$  terms  $x''_i x_j + x_i x''_j$  for which  $1 \leq i \leq v, d + 1 \leq j \leq n$ , and  $i < j$ . Thus  $\alpha \geq rx''_1(x_{d-1} + x_d) \geq 2rx''_1 x_{d+1} \geq (r + t)x''_1 x_{d+1} \geq \beta$ , establishing the required inequality.

Turning now to subcase (IIb), suppose first that  $n \geq d + 2$  and  $a_{1,d+2} = 1$ , and let  $h$  be maximal such that  $a_{h,d+2} = 1$ . Note that  $h \leq t - 2$  because  $a_{t+1,d+1} = 1$  and  $r < t$ . Let  $a = t - h$  and  $b = v - t$ . Let  $k$  be maximal such that  $a_{hk} = 1$ , and let  $q$  be minimal such that  $a_{v+1,q} = 0$  and  $v + 1 < q$ . The numbers  $a, b, d, h, k, q, t, v$  are illustrated in Figure 2 for a typical matrix  $A' - A$ : in the illustration,  $q \leq d$ , but the arguments which follow embrace also the case  $q = d + 1$ . Invoking property  $(**)$  with  $p = v + 1$ , we have  $v + q \leq h + k$ ; equivalently  $[k - (d + 1)] + [d - (q - 1)] \geq a + b$ . Suppose by way of contradiction that  $d - (q - 1) < b$ : then  $k - (d + 1) \geq a + 1$ . But  $t - 1 \geq r \geq b + [k - (d + 1)]h$ , and it follows that  $t - 1 \geq b + (a + 1)(t - a)$ , whence  $t \leq a + 1 - (b + 1)a^{-1}$  and  $h \leq 0$ , a contradiction. Hence  $d - (q - 1) \geq b$ : therefore,  $v \leq d - b - 1$ , and we can define the matrix  $A'' = (a''_{ij}) \in \mathcal{S}^*(n, e)$  as follows. For  $i < j$  we have  $a''_{ij} = 1$  precisely when  $j \leq d - 1$ , or  $j = d$  and  $1 \leq i \leq d - b - 1$ , or  $j = d + 1$  and  $1 \leq i \leq v$ . The matrix  $A''$  is illustrated in Figure 3.

Let  $\rho'' = \rho(A'')$  with corresponding nonnegative unit eigenvector  $x'' = (x''_1, \dots, x''_n)^T$ , and let  $w = d - b - 1 - v$ . The equations (I) yield the following in respect of  $A''$ :

$$(\rho'' + 1)x''_1 = vx''_1 + wx''_{d-b-1} + x''_{d-1} + x''_d + x''_{d+1},$$

$$(\rho'' + 1)x''_{d-1} = vx''_1 + wx''_{d-b-1} + bx''_{d-1},$$

$$\rho'' x''_d = vx''_1 + wx''_{d-b-1}.$$

We deduce that  $x''_{d-1} + x''_d > x''_1$ . Now  $x^T x''(\rho'' - \rho) = \alpha - \beta$ , where  $\alpha$  is the sum of (say)  $r'$  terms  $x''_i x_j + x_i x''_j$  for which  $i < j \leq d$ , and  $\beta$  is a sum of  $r'$  terms  $x''_i x_j + x_i x''_j$  for which  $j \geq d + 2$  and  $i < j$ . Hence  $\alpha \geq r'(x''_{d-1} x_d + x''_d x_{d-1}) \geq r' x_d (x''_{d-1} + x''_d) > r' x''_1 x_d \geq r' x''_1 x_{d+2}$ . On the other hand,  $x''_j = 0$  for  $j \geq d + 2$  and so  $\beta \leq r' x''_1 x_{d+2}$ , whence  $\rho < \rho''$ .

	(g)	(d)	(k)	
	0 0 .....	0 0 -1 .....	-1 *	
	· · ·	· · ·	· · ·	
	· · ·	· · ·	· · ·	
(h)	0 0 .....	0 0 -1 .....	-1 0	
	0 0 .....	0 0 0 .....	0 0	}
	· · ·	· · ·	· · ·	
	· · ·	· · ·	· · ·	
(t)	0 0 .....	0 0 0 .....	0 0	}
	0 0 .....	0 -1 0 .....	0 0	
	· · ·	· · ·	· · ·	
(v)	0 0 .....	0 -1 0 .....	0 0	}
	0 1 .....	1 0 0 .....	0 0	
	* 1 .....	1 0 0 .....	0 0	
	· · ·	· · ·	· · ·	
	· · ·	· · ·	· · ·	
	1 .....	1 0 0 .....	0 0	
(g)	0	· · ·	· · ·	
		· · ·	· · ·	
		· · ·	· · ·	
		· · ·	· · ·	
		· · ·	· · ·	
		1 0 0 .....	0 0	
(d)		0 0 0 .....	0 0	
		0 0 .....	0 0	

FIG. 2. Part of the matrix  $A' - A$ , subcase *IIb*.



					(d)			(r)				
	0	1	1	.....	1	1	1	0	.....	0	}	$t + b$
		0	1	.....	1	1	1	0	.....	0		
					.	.	.	.		.		
					.	.	.	.		.		
(v)					1	1	1	0	.....	0	}	$b$
					1	1	0	0	.....	0		
					.	.	.	.		.		
					.	.	.	.	.....	0		
(d-b-1)					1	1	0	0	.....	0	}	$b$
					1	0	0	0	.....	0		
					.	.				.		
					.	.				.		
					1	0	0	0	.....	0	}	$b$
					0	0	0	0	.....	0		
(d)					0	0	0	.....	0	0		

FIG. 3. Part of the matrix  $A''$ , subcase  $IIb$ .

If  $A'' \notin \mathcal{S}^{**}(n, e)$  (equivalently, if  $d - t - 2b \geq 3$ ), then  $\rho'' < \rho'$  because the spectral radius of  $A''$  may be increased by successively transferring the last  $b$  entries equal to 1 in column  $d + 1$  to positions  $(i, d)$  ( $i = d - b, \dots, d - 1$ ) as in the proof of Lemma 2. Thus  $\rho < \rho'$  when  $A'' \notin \mathcal{S}^{**}(n, e)$ . If  $A'' \in \mathcal{S}^{**}(n, e)$ , then  $A''$  is an instance of a matrix  $A$  in  $\mathcal{S}^{**}(n, e)$  for which  $a_{1, d+2} = 0$ . Accordingly, to prove that  $\rho < \rho'$  in every case it suffices to prove that  $\rho(A) < \rho'$  for those matrices  $A = (a_{ij}) \in \mathcal{S}^{**}(n, e) - \{A'\}$  for which  $a_{1, d+2} = 0$  and  $b = r < t$ . Since isolated vertices of the corresponding graphs may be ignored, we may assume that  $n = d + 1$ .

We now have  $x_1 = \dots = x_{t+b}$ ,  $t + b < d$  and  $\rho x_{d+1} = (t + b)x_1$ . Moreover  $x^T x'(\rho' - \rho) = \alpha - \beta$ , where  $\alpha$  is the sum of  $b$  terms  $x'_i x_j + x_i x'_j$  with  $i < j \leq d$ , and  $\beta = x_{d+1}(x'_{t+1} + \dots + x'_{t+b}) + x'_{d+1}(x_{t+1} + \dots + x_{t+b})$ . Hence  $\alpha \geq b(x'_{d-1} x_d + x_{d-1} x'_d) = b x'_d (x_d + x_{d-1})$  and  $\beta = b(x_{d+1} x'_d + x'_{d+1} x_1)$ . Thus  $\alpha - \beta \geq b\{x'_d(x_d + x_{d-1} - x_{d+1}) - x'_{d+1} x_1\}$ , and it suffices to

prove that

$$\frac{x'_d}{x'_{d+1}} > \frac{x_1}{x_d + x_{d-1} - x_{d+1}}.$$

Since  $\{\rho' - (d - 1 - t)\}x'_d = tx'_1 = \rho'x'_{d+1}$ , we have

$$\frac{x'_d}{x'_{d+1}} = \frac{\rho'}{\rho' - (d - 1 - t)}.$$

On the other hand,  $\rho(x_d + x_{d-1} - x_{d+1}) \geq \rho x_d \geq \rho x_{d+1} = (t + b)x_1$ , and so

$$\frac{x_1}{x_d + x_{d-1} - x_{d+1}} \leq \frac{\rho}{t + b} < \frac{d}{t + b}.$$

Hence it suffices to prove that

$$\frac{\rho'}{\rho' - (d - 1 - t)} \geq \frac{d}{t + b}$$

—equivalently, that

$$\rho' \leq d \left( \frac{d - t - 1}{d - t - b} \right).$$

This is clear because  $\rho' < d$ , and the Theorem is now proved. ■

We now know that when

$$e = \binom{d}{2} + t, \quad 0 < t < d,$$

the graph  $G_e$  has the largest index of any graph in  $\mathcal{S}(e)$ : accordingly  $f(e)$  is the largest eigenvalue of the matrix

$$\begin{pmatrix} t-1 & d-t & 1 \\ t & d-t-1 & 0 \\ t & 0 & 0 \end{pmatrix}.$$

Hence  $f(e) = d - 1 + \varepsilon$ , where  $0 < \varepsilon < 1$  and  $\varepsilon^3 + (2d - 1)\varepsilon^2 + (d^2 - d - t)\varepsilon - t^2 = 0$ .

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