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Discrete Applied Mathematics 127 (2003) 615–626
DISCRETE APPLIED MATHEMATICS
www.elsevier.com/locate/dam

Maximal value of the zeroth-order Randić index

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Received 5 July 2000; received in revised form 27 April 2001; accepted 10 December 2001

Abstract

Let $G(n,m)$ be a connected graph without loops and multiple edges which has n vertices and m edges. We find the graphs on which the zeroth-order connectivity index, equal to the sum of degrees of vertices of $G(n,m)$ raised to the power $-\frac{1}{2}$, attains maximum.

MSC: 05C35

Keywords: Extremal graph; Zeroth-order connectivity index

1. Introduction

Let $G(n,m)$ be a connected graph without loops and multiple edges which has n vertices and m edges. Denote by u its vertex and by δ_u the degree of the vertex u, that is the number of edges of which u is an endpoint. Denote further by (uv) the edge whose endpoints are the vertices u and v. In 1975 Randić proposed a topological index, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The Randić index defined in [9] is: $\chi=\sum_{(uv)}(\delta_u\delta_v)^{-1/2}$, where the summation goes over all edges of G. Randić himself demonstrated [9] that his index is well correlated with a variety of physico-chemical properties of alcanes. χ became one of the most popular molecular descriptors to which two books are devoted [6,8]. The general Randić index w_α is $w_\alpha=\sum_{(uv)}(\delta_u\delta_v)^\alpha$, where the summation goes over all edges of G. The zeroth-order Randić index ${}^0\chi$ defined by Kier and Hall [7,8] is

$$ {}^0\chi=\sum_{(u)}(\delta_u)^{-1/2}, $$

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0166-218X/03/$ - see front matter
PII: S0166-218X(02)00392-X

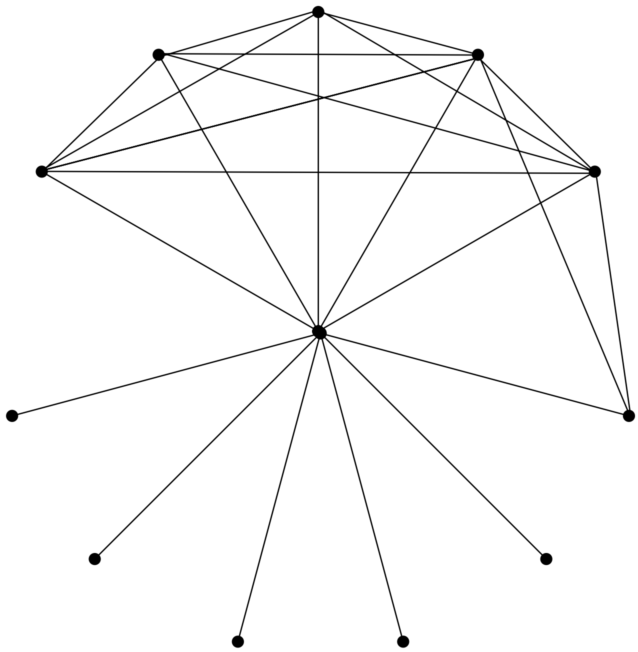

Fig. 1. Extremal graph $G(12,23)$, $n_1=5, n_3=1, n_5=3, n_6=2, n_{11}=1$.

where the summation goes over all vertices of G. Kier and Hall gave a general scheme based on the Randić index to calculate also zeroth-order ${}^0\chi$ and higher-order connectivity indices ${}^m\chi$. For example, the second order connectivity index is: ${}^2\chi = \sum_{(uvw)} (\delta_u\delta_v\delta_w)^{-1/2}$, where the summation goes over all paths of length 2. Initially, the Randić connectivity index was studied only by chemists [7,8], but recently it attracted the attention also of mathematicians [1,2,4,5]. In [3] the general Randić index has been studied for $\alpha = -1$, that is the former index proposed by Randić. One of the most obvious mathematical questions to be asked in connection with ${}^m\chi$ is which graphs (from a given class) have maximum and minimum ${}^m\chi$ values [1]. These questions are interesting for chemists too, because there is a connection between connectivity indices and some physico-chemical properties for "chemical graphs". The solution of such problems turned out to be difficult, and only a few partial results have been achieved so far.

Denote by n_i the number of vertices of degree i. Then: ${}^0\chi = n_1/\sqrt{1} + n_2/\sqrt{2} + \cdots + n_{n-1}/\sqrt{n-1}$. The function ${}^0\chi$ attains maximum on the following connected graphs. For $m=n-1$, it is a star graph, then we add a new edge (for $m=n$) between two vertices of degree 1 and get a clique of 3 vertices. Adding one more edge (for $m=n+1$) between one vertex out of the clique and some vertices in the clique increases the degree of this vertex by 1 until it is joined to all those of the clique. We get a clique of 4 vertices ($m=n+2$) and we continue to add edges in this manner until we arrive at the complete graph (Fig. 1). Denote by $G^* = G^*(n,m)$ the graph on which ${}^0\chi$ attains maximum.

Theorem. *Let $G(n,m)$ be a connected graph without loops and multiple edges with n vertices and m edges. If $m=n+k(k-3)/2+p$, where $2 \leqslant k \leqslant n-1$ and $0 \leqslant p \leqslant k-2$, then*

$$^0\chi(G(n,m)) \leqslant {}^0\chi(G^*) = \frac{n-k-1}{\sqrt{1}} + \frac{1}{\sqrt{p+1}} + \frac{k-1-p}{\sqrt{k-1}} + \frac{p}{\sqrt{k}} + \frac{1}{\sqrt{n-1}}. \quad (1)$$

It means that the extremal graph above described, must have $n_1 = n-k-1$, $n_{p+1}=1$, $n_{k-1} = k-1-p$, $n_k = p$ and $n_{n-1} = 1$.

The theorem describes the solution of the following problem (P):

$$\max \frac{n_1}{\sqrt{1}} + \frac{n_2}{\sqrt{2}} + \frac{n_3}{\sqrt{3}} + \cdots + \frac{n_{n-1}}{\sqrt{n-1}}$$

under two graph constraints:

$$n_1 + n_2 + n_3 + \cdots + n_{n-1} = n, \quad (A)$$

$$n_1 + 2n_2 + 3n_3 + \cdots + (n-1)n_{n-1} = 2m. \quad (B) \quad (B)$$

It is not difficult to prove the theorem for trees.

Lemma 1. *If $m = n-1$, the function $^0\chi$ attains maximum on the star graph.*

Proof. When $m = n-1$, then $k = 2$ and $p = 0$. We find n_1 and n_{n-1} from constraints (A) and (B)

$$n_1 = n - 1 - \left(1 - \frac{1}{n-2}\right) n_2 - \left(1 - \frac{2}{n-2}\right) n_3 - \cdots - \left(1 - \frac{n-3}{n-2}\right) n_{n-2},$$

$$n_{n-1} = 1 - \frac{n_2}{n-2} - \frac{2n_3}{n-2} - \frac{3n_4}{n-2} - \cdots - \frac{(n-3)n_{n-2}}{n-2}.$$

After their substitution in $^0\chi$, this function becomes

$$^0\chi = n - 1 + \frac{1}{\sqrt{n-1}} + \sum_{j=2}^{n-2} \left(\frac{1}{\sqrt{j}} - \frac{n-1-j}{n-2} - \frac{j-1}{(n-2)\sqrt{n-1}} \right) n_j.$$

Since (see Lemma 2): $(n-2)/\sqrt{j} \leqslant (n-1-j)/\sqrt{1} + (j-1)/\sqrt{n-1}$ for $1 \leqslant j \leqslant n-1$, we conclude that $^0\chi$ attains maximum for $n_j = 0$, $j = 2, 3, \ldots, n-2$. Then: $n_1 = n-1, n_2 = n_3 = \cdots = n_{n-2} = 0$, $n_{n-1} = 1$ and $\max_{m=n-1} {}^0\chi = n - 1 + 1/\sqrt{n-1}$. □

Lemma 2. *Let r, s, and t be real numbers such that*: $0 < r \leqslant s \leqslant t$. *Then*

$$\frac{t-r}{\sqrt{s}} \leqslant \frac{t-s}{\sqrt{r}} + \frac{s-r}{\sqrt{t}}$$

and the equality holds only for $s = r$ and t.

Proof. If $s=r$ or $s=t$, it is obvious that equality holds. Denote by $f(s)=(t-s)/\sqrt{r}+(s-r)/\sqrt{t}-(t-r)/\sqrt{s}$. Then $\partial^2 f/\partial s^2=-\frac{3}{4}(t-r)s^{-5/2}<0$ and the upper inequality follows because the function f is strictly concave. □

Corollary 1. *For real number s, such that* $s>1$, *holds*:

$$\frac{2}{\sqrt{s}}<\frac{1}{\sqrt{s-1}}+\frac{1}{\sqrt{s+1}}.$$

If we want to find extremal graphs for other values of m we cannot use the same method because the solutions do not correspond to graphs.

The proof of the following lemma is easy and is omitted.

Lemma 3. *If* $n_1\neq 0$ *in* $G(n,m)$, *then* $n_{n-1}\leqslant 1$. *If* $n_1=n_2=\cdots=n_{i-1}=0$ *and* $n_i\neq 0$ *then* $n_{n-1}\leqslant i$.

Lemma 4. *If* $n_{n-1}=1$ *and* $n_1=l$ $(l\geqslant 2)$ *in* $G(n,m)$, *then* $n_{n-l}=n_{n-l+1}=\cdots=n_{n-3}=n_{n-2}=0$.

Proof. Consider a vertex of degree k $(k>1)$. Since l vertices of degree 1 are adjacent to the vertex of degree $n-1$, this vertex can be adjacent to the most $n-1-l$ other vertices. It means that $k\leqslant n-l-1$. □

When $n_{n-1}=1$ and $n_1=l$, instead of problem (P) we can consider the following problem (P^l):

$$\max\frac{l}{\sqrt{1}}+\frac{n_2}{\sqrt{2}}+\frac{n_3}{\sqrt{3}}+\cdots+\frac{n_{n-l-1}}{\sqrt{n-l-1}}+\frac{1}{\sqrt{n-1}}$$

under the constraints:

$$n_2+n_3+n_4+\cdots+n_{n-l-1}=n-1-l, \tag{A^1}$$

$$n_2+2n_3+3n_4+\cdots+(n-l-2)n_{n-l-1}=2(m-n+1). \tag{B^1}$$

2. The main part of the proof

The proof of the theorem is based on mathematical induction. It is easy to check that the theorem is true for $n=5$ and $4\leqslant m\leqslant 10$. We will suppose that the theorem is true for every graph $G(i,j)$, where $5\leqslant i\leqslant n-1$ and $i-1\leqslant j\leqslant\binom{i}{2}$. We have to prove the theorem for graphs $G(n,m)$, where $n-1\leqslant m\leqslant\binom{n}{2}$. The case $m=n-1$ is done and the cases $m=\binom{n}{2}$ and $\binom{n}{2}-1$ will not be considered because they correspond to unique graphs. Since $m=n+k(k-3)/2+p$, where $2\leqslant k\leqslant n-1$ and $0\leqslant p\leqslant k-2$, we need to consider two cases: (1) $k=n-1$ and (2) $2\leqslant k\leqslant n-2$. At first, we will prove the theorem for $k=n-1$.

Case 1: $k=n-1$.

Lemma 5. *Inequality* (1) *holds for the graphs* $G(n,m)$, $m=n+k(k-3)/2+p$, where $k=n-1$ and $0 \leqslant p \leqslant n-3$.

Proof. The number of edges is $m=(n^2-3n+4+2p)/2=(n-1)(n-2)/2+p+1$, where $0 \leqslant p \leqslant n-3$. If $p \geqslant 1$, then $n_1=n_2=n_3=\cdots=n_p=0$ and $n_{p+1} \geqslant 0$. Contrary to this, if $G(n,m)$ would have one vertex of degree p (or less), by deleting one vertex of degree p we get the graph $G'(n-1,m-p)$ (not necessarily connected), which has more edges than the complete graph on $n-1$ vertices. The fact that $n_{p+1} \geqslant 0$ means: $n_{p+1} \neq 0$ or $n_{p+1}=0, n_{p+2} \neq 0$ or $n_{p+1}=n_{p+2}=0, n_{p+3} \neq 0$ and so on. Denote by P_p^{p+j+1} the problem for given p when $n_1=n_2=\cdots=n_p=n_{p+1}=n_{p+2}=\cdots=n_{p+j}=0$, $n_{p+j+1} \neq 0$ and by ${}^0\chi_p^{p+j+1}$ the optimal value of ${}^0\chi$ for the problem P_p^{p+j+1}. The optimal value of ${}^0\chi$ for given p is ${}^0\chi_p = \max_{0 \leqslant j \leqslant n-p-4} {}^0\chi_p^{p+j+1}$. When we have $n_{p+j+1} \neq 0$, then $n_{n-1} \leqslant p+j+1$ (Lemma 3).

Let us solve the problem P_p^{p+j+1}, $0 \leqslant p \leqslant n-4$, $0 \leqslant j \leqslant n-p-4$. (When $p=n-3$, we have only one graph, that is the complete graph without one edge.)

$$\max \frac{n_{p+j+1}}{\sqrt{p+j+1}} + \frac{n_{p+j+2}}{\sqrt{p+j+2}} + \frac{n_{p+j+3}}{\sqrt{p+j+3}} + \cdots + \frac{n_{n-1}}{\sqrt{n-1}}$$

under the constraints:

$$n_{p+j+1} + n_{p+j+2} + n_{p+j+3} + \cdots + n_{n-1} = n,$$

$$(p+j+1)n_{p+j+1} + (p+j+2)n_{p+j+2} + \cdots + (n-1)n_{n-1} = n^2-3n+4+2p,$$

$$n_{n-1} = p+j+1-\xi.$$

Let us solve the system of the latter three equalities in n_{n-1}, n_{n-2} and n_{p+j+1}

$$\begin{aligned} n_{n-2} = {} & \frac{n^2-n(2p+2j+5)+p^2+2pj+5p+j^2+3j++6}{n-p-j-3} - \frac{n_{p+j+2}}{n-p-j-3} \\ & - \frac{2n_{p+j+3}}{n-p-j-3} - \frac{3n_{p+j+4}}{n-p-j-3} \\ & - \cdots - \frac{(n-p-j-4)n_{n-3}}{n-p-j-3} - \frac{(n-p-j-2)\xi}{n-p-j-3}, \end{aligned}$$

$$\begin{aligned} n_{p+j+1} = {} & \frac{n-p+j-3}{n-p-j-3} - \left(1-\frac{1}{n-p-j-3}\right) n_{p+j+2} \\ & - \left(1-\frac{2}{n-p-j-3}\right) n_{p+j+3} - \left(1-\frac{3}{n-p-j-3}\right) n_{p+j+4} \\ & - \cdots - \left(1-\frac{n-p-j-4}{n-p-j-3}\right) n_{n-3} + \left(1-\frac{n-p-j-2}{n-p-j-3}\right) \xi. \end{aligned}$$

After substituting n_{p+j+1}, n_{n-2} and n_{n-1} back into ${}^0\chi$, we have

$$
\begin{aligned}
{}^0\chi = {} & \frac{n-p+j-3}{(n-p-j-3)\sqrt{p+j+1}} \\
& + \frac{n^2-n(2p+2j+5)+p^2+2pj+5p+j^2+3j+6}{(n-p-j-3)\sqrt{n-2}} + \frac{p+j+1}{\sqrt{n-1}} \\
& + \sum_{i=p+j+2}^{n-3} n_i \left(\frac{1}{\sqrt{i}} - \frac{n-i-2}{(n-p-j-3)\sqrt{p+j+1}} - \frac{i-p-j-1}{(n-p-j-3)\sqrt{n-2}} \right) \\
& + \xi \left(-\frac{1}{\sqrt{n-1}} - \frac{1}{(n-p-j-3)\sqrt{p+j+1}} + \frac{n-p-j-2}{(n-p-j-3)\sqrt{n-2}} \right).
\end{aligned}
$$

Since (because of Lemma 2)

$$
\frac{n-p-j-3}{\sqrt{i}} \leqslant \frac{n-i-2}{\sqrt{p+j+1}} + \frac{i-p-j-1}{\sqrt{n-2}} \quad \text{for } p+j+1 \leqslant i \leqslant n-2,
$$

$$
\frac{n-p-j-2}{\sqrt{n-2}} \leqslant \frac{1}{\sqrt{p+j+1}} + \frac{n-p-j-3}{\sqrt{n-1}}.
$$

The latter inequality is obtained for $i = n-2$ from the inequality

$$
\frac{n-p-j-2}{\sqrt{i}} \leqslant \frac{n-i-1}{\sqrt{p+j+1}} + \frac{i-p-j-1}{\sqrt{n-1}} \quad \text{for } p+j+1 \leqslant i \leqslant n-1.
$$

It means that we will get the maximum value of ${}^0\chi$ if we put: $n_{p+j+2} = n_{p+j+3} = \cdots = n_{n-3} = \xi = 0$ and

$$
\begin{aligned}
{}^0\tilde{\chi}_p^{p+j+1} = {} & \frac{n-p+j-3}{(n-p-j-3)\sqrt{p+j+1}} \\
& + \frac{n^2-n(2p+2j+5)+p^2+2pj+5p+j^2+3j+6}{(n-p-j-3)\sqrt{n-2}} + \frac{p+j+1}{\sqrt{n-1}}
\end{aligned}
$$

for $p = 0, 1, \ldots, n-4$ and $j = 0, 1, \ldots, n-p-4$. This solution does not correspond always to a graph (except for $j=0$, ${}^0\tilde{\chi}_p^{p+1} = {}^0\chi_p^{p+1}$). We put symbol $\sim$ for this solution, but the true graph solution ${}^0\chi_p^{p+j+1}$ is less than or equal to ${}^0\tilde{\chi}_p^{p+j+1}$.

Now we show that ${}^0\chi_p^{p+1}$ is the maximum value of ${}^0\chi$ for a given number p, that is, ${}^0\chi_p^{p+1} = \max_{0 \leqslant j \leqslant n-p-4} {}^0\chi_p^{p+j+1}$. Since ${}^0\chi_p^{p+j+1} \leqslant {}^0\tilde{\chi}_p^{p+j+1}$, it is sufficient to prove that $\chi_p^{p+1} = \max_{0 \leqslant j \leqslant n-p-4} {}^0\tilde{\chi}_p^{p+j+1}$. We have to prove the following inequality:

$$
{}^0\tilde{\chi}_p^{p+j+1} \leqslant \frac{1}{\sqrt{p+1}} + \frac{n-p-2}{\sqrt{n-2}} + \frac{p+1}{\sqrt{n-1}}. \tag{5}
$$

We transform inequality (5) (for $n-p-j-3 \neq 0$) to (6)

$$
\frac{n-p-j-3}{\sqrt{p+1}} - \frac{n-p+j-3}{\sqrt{p+j+1}} + \frac{j(n-p-j-1)}{\sqrt{n-2}} - \frac{j(n-p-j-3)}{\sqrt{n-1}} \geqslant 0. \tag{6}
$$

We introduce the abbreviations: $A=\sqrt{p+1}$, $B=\sqrt{p+j+1}$, $C=\sqrt{n-1}$ and $D=\sqrt{n-2}$ in order to facilitate writing. After this, inequality (6) becomes

$$j\left\{\frac{n-p-j-3}{AB[A+B]}-\frac{n-p-j-3}{CB[C+B]}+\frac{n-p-j-1}{CD[C+D]}-\frac{n-p-j-1}{CB[C+B]}\right\}\geqslant 0 \quad (7)$$

which is transformed into

$$\frac{j(n-p-j-3)}{BC(B+C)}\left\{\frac{(n-p-2)(A+B+C)}{A(A+B)(A+C)}\right.$$
$$\left.-\frac{(n-p-j-1)(B+C+D)}{D(B+D)(C+D)}\right\}\geqslant 0. \quad (8)$$

This inequality holds for $j=0,1,\ldots,n-p-4$ and for $p=0,1,\ldots,n-4$ because $n-p-2\geqslant n-p-j-1$ for $j\geqslant 1$ (for $j=0$ in (8) holds equality) and

$$\frac{A+B+C}{A(A+B)(A+C)}>\frac{B+C+D}{D(B+D)(C+D)}. \quad (9)$$

Since $A<D$, follows: $1/(A+B)>1/(B+D)$ and $1/(A+C)>1/(C+D)$, and (9) becomes $(A+B+C)/A>(B+C+D)/D$. The last inequality is true again because $A<D$.

We proved that the maximum value of ${}^0\chi$ for a given number p is ${}^0\chi_p^{p+1}$

$${}^0\chi_p^{p+1}=\frac{1}{\sqrt{p+1}}+\frac{n-p-2}{\sqrt{n-2}}+\frac{p+1}{\sqrt{n-1}}$$

for $p=0,1,\ldots,n-4$. This value is attained on a graph which has $n_{n-1}=p+1$, $n_{n-2}=n-p-2$ and $n_{p+1}=1$. □

Case 2: $2\leqslant k\leqslant n-2$.

Now we will consider the graphs $G(n,m)$, where $m=n+k(k-3)/2+p$ and $2\leqslant k\leqslant n-2$ and $0\leqslant p\leqslant k-2$. We will prove that G^* has at least one vertex of degree $n-1$.

Lemma 6. *Let $n-t$ $(t\geqslant 2)$ be the maximum degree and l be the minimum degree of the vertices in G^*. Then every vertex of the minimum degree l must be adjacent to every vertex of the maximum degree $n-t$.*

Proof. Suppose the opposite, namely, that there exists a vertex u of degree l which is not adjacent to a vertex w of the maximum degree. Denote by G' a graph obtained from G^* by deleting an edge between vertex u and some vertex v of degree j $(l\leqslant j\leqslant n-t)$ and joining the vertices u and w with a new edge. Then

$$\begin{aligned}{}^0\chi(G')-{}^0\chi(G^*)&=\frac{1}{\sqrt{n-t+1}}-\frac{1}{\sqrt{n-t}}+\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\\&\geqslant\frac{1}{\sqrt{n-t+1}}-\frac{1}{\sqrt{n-t}}+\frac{1}{\sqrt{n-t-1}}-\frac{1}{\sqrt{n-t}}>0\end{aligned}$$

because the function $1/\sqrt{j-1}-1/\sqrt{j}$ is decreasing and because of Corollary 1. □

Lemma 7. *The minimum degree of vertices in* G^* *which has the maximum degree* $n-t$, $t \geqslant 2$ *is* 1.

Proof. Suppose the opposite, namely, that the minimum degree of vertices in G^* is l, $l \geqslant 2$. A vertex u of degree l is adjacent to one vertex of the maximum degree and to other vertex v. Denote by G' a graph obtained from G^* when we delete the edge between vertices u and v and introduce a new edge between vertex v and a vertex w of degree j ($l \leqslant j \leqslant n-t$). We can always do this because the degree k of v: $k \leqslant n-t < n-1$ and there exists at least one vertex w which is not adjacent to vertex v. Then

$$
\begin{aligned}
{}^0\chi(G') - {}^0\chi(G^*) &= \frac{1}{\sqrt{l-1}} - \frac{1}{\sqrt{l}} + \frac{1}{\sqrt{j+1}} - \frac{1}{\sqrt{j}} \\
&\geqslant \frac{1}{\sqrt{l-1}} - \frac{1}{\sqrt{l}} + \frac{1}{\sqrt{l+1}} - \frac{1}{\sqrt{l}} > 0
\end{aligned}
$$

because the function $1/\sqrt{j+1} - 1/\sqrt{j}$ is increasing and because of Corollary 1. □

Lemma 8. *The extremal graph* G^* *must have at least one vertex of degree* $n-1$.

Proof. Suppose the contrary, that is, that the maximum degree of the vertices is $n-t$ ($t \geqslant 2$). As we showed, all vertices of degree 1 must be adjacent to one vertex w of degree $n-t$. Denote by G' a graph obtained from G^* when we delete one vertex of degree 1. The graph $G'(n', m')$ has $n' = n-1$ vertices and $m' = m-1$ edges (for $k \leqslant n-2$) and for it inductive hypothesis holds

$$
{}^0\chi(G') \leqslant \frac{n-1-k-1}{\sqrt{1}} + \frac{1}{\sqrt{p+1}} + \frac{k-1-p}{\sqrt{k-1}} + \frac{p}{\sqrt{k}} + \frac{1}{\sqrt{n-2}}
$$

and

$$
\begin{aligned}
{}^0\chi(G^*) &= {}^0\chi(G') + \frac{1}{\sqrt{1}} + \frac{1}{\sqrt{n-t}} - \frac{1}{\sqrt{n-t-1}} \\
&\leqslant \frac{n-1-k}{\sqrt{1}} + \frac{1}{\sqrt{p+1}} + \frac{k-1-p}{\sqrt{k-1}} + \frac{p}{\sqrt{k}} \\
&\quad + \frac{1}{\sqrt{n-2}} + \frac{1}{\sqrt{n-t}} - \frac{1}{\sqrt{n-t-1}} \\
&< \frac{n-1-k}{\sqrt{1}} + \frac{1}{\sqrt{p+1}} + \frac{k-1-p}{\sqrt{k-1}} + \frac{p}{\sqrt{k}} + \frac{1}{\sqrt{n-1}}
\end{aligned}
$$

because $1/\sqrt{n-2} - 1/\sqrt{n-1} < 1/\sqrt{n-t-1} - 1/\sqrt{n-t}$. It means that : ${}^0\chi(G^*) < (n-1-k)/\sqrt{1} + 1/\sqrt{p+1} + (k-1-p)/\sqrt{k-1} + p/\sqrt{k} + 1/\sqrt{n-1}$, which is impossible. ${}^0\chi$ attains this value on a graph which has $n_1 = n-k-1$, $n_{p+1} = 1$, $n_{k-1} = k-p-1$, $n_k = p$ and $n_{n-1} = 1$. □

Subcase 2a: $2 \leqslant k \leqslant n-2$, $n_1 \neq 0$.

First, we consider the extremal graphs which have $n_1 \neq 0$. Then $n_{n-1} = 1$ (Lemmas 3 and 8) and all vertices of degree 1 must be adjacent to this unique vertex of degree $n-1$.

Lemma 9. *Inequality* (1) *holds for all graphs* $G(n,m)$, $n_{n-1}=1$, $n_1=l$, $(l \geqslant 1)$ *and for* $2 \leqslant k \leqslant n-2$.

Proof. Inequality (1) will be valid for all graphs $G(n,m)$, $n_{n-1}=1$ and $n_1=l$, if the following inequality holds:

$$\frac{n_2}{\sqrt{2}}+\frac{n_3}{\sqrt{3}}+\cdots+\frac{n_{n-l-1}}{\sqrt{n-l-1}} \leqslant \frac{n-k-1-l}{\sqrt{1}}+\frac{1}{\sqrt{p+1}}+\frac{k-1-p}{\sqrt{k-1}}+\frac{p}{\sqrt{k}} \tag{2}$$

under constraints: (A^1) and (B^1). We first prove (2) for $l \geqslant 2$. Consider a graph $G'(n-1,m-1)$, which is obtained from $G(n,m)$, when we delete one vertex of degree 1. The graph $G'(n-1,m-1)$ has $n'_1=l-1$ and one vertex of degree $n-2$ (because the other vertices can have degree at the most $n-1-l$), and we can use Lemma 4. Namely, when $n'_1=l-1$, then $n'_{n-l}=n'_{n-l+1}=\cdots=n'_{n-3}=0$ (because $n-1-(l-1)=n-l$) and the same constraints: (A^1) and (B^1) hold. Since $G'(n-1,m-1)$ has $n-1$ vertices and $n-1+k(k-3)/2+p$ edges, it satisfies the inductive hypothesis. Holds

$$\frac{n_2}{\sqrt{2}}+\frac{n_3}{\sqrt{3}}+\cdots+\frac{n_{n-l-1}}{\sqrt{n-l-1}} \leqslant \frac{n-1-k-1-(l-1)}{\sqrt{1}}+\frac{1}{\sqrt{p+1}}+\frac{k-1-p}{\sqrt{k-1}}+\frac{p}{\sqrt{k}} \tag{2'}$$

for every $2 \leqslant k \leqslant n-2$ and $0 \leqslant p \leqslant k-2$. We omitted the symbol$'$, but all denotations pertain to G'. Inequality (2$'$) is just inequality (2), which is now proved because the constraints are the same.

Now we show that inequality (2) holds for $l=1$, that is, when the graph G' has no vertex of degree one. Since $n_{n-2} \geqslant 1$ in the graph $G'(n-1,m-1)$, we can introduce the following substitution: $n_{n-2}=1+n'_{n-2}$. By the inductive hypothesis for the graph G' holds

$$\frac{n_2}{\sqrt{2}}+\frac{n_3}{\sqrt{3}}+\cdots+\frac{n_{n-2}}{\sqrt{n-2}} \leqslant \frac{n-1-k-1}{\sqrt{1}}+\frac{1}{\sqrt{p+1}}+\frac{k-1-p}{\sqrt{k-1}}+\frac{p}{\sqrt{k}}+\frac{1}{\sqrt{n-2}} \tag{3}$$

under the costraints

$$n_2+n_3+\cdots+n_{n-2}=n-1,$$

$$2n_2+3n_3+\cdots+(n-2)n_{n-2}=2(m-1). \tag{4}$$

After this substitution inequality (3) and system of equalities (4) becomes (3′) and (4′). Namely, it holds

$$\frac{n_2}{\sqrt{2}} + \frac{n_3}{\sqrt{3}} + \cdots + \frac{n_{n-3}}{\sqrt{n-3}} + \frac{n'_{n-2}}{\sqrt{n-2}}$$
$$\leqslant \frac{n-1-k-1}{\sqrt{1}} + \frac{1}{\sqrt{p+1}} + \frac{k-1-p}{\sqrt{k-1}} + \frac{p}{\sqrt{k}} \tag{3'}$$

under the costraints

$$n_2 + n_3 + \cdots + n_{n-3} + n'_{n-2} = n-2,$$
$$n_2 + 2n_3 + \cdots + (n-4)n_{n-3} + (n-3)n'_{n-2} = 2(m-n+1). \tag{4'}$$

Equalities (4′) are just the constraints: (A^1), (B^1) and inequality (3′) is inequality (2) for $l=1$. □

Subcase 2b: $2 \leqslant k \leqslant n-2$, $n_1 = 0$.

We will now consider the case when $n_1 = 0$. The proofs of the next two Lemmas 10 and 11 are similar to those of Lemmas 6 and 7 and are omitted.

Lemma 10. *Let* $n_1 = n_2 = \cdots = n_{r-1} = 0$, $n_r \neq 0$ $(r \geqslant 2)$ *in the extremal graph* G^* *and* $n-1 \geqslant n-t_1 \geqslant n-t_2 \geqslant \cdots \geqslant n-t_{r-1}$ *be the first r maximum degrees of vertices. Then every vertex of degree r must be adjacent to every vertex of these maximum degrees.*

Lemma 11. *If in* G^*, $n_1 = n_2 = \cdots = n_{r-1} = 0$ *and* $n_r \neq 0$, *then the extremal graph* G^* *has r vertices of degree* $n-1$.

Earlier we proved the theorem for $k = n-1$, namely when the number of edges $m \geqslant (n^2-3n+4)/2$. It remains to prove the theorem when $m < (n^2-3n+4)/2$.

Lemma 12. *If* $m \leqslant (n^2-3n+2)/2$ *then the extremal graph* G^*, *such that*: $n_1 = n_2 = \cdots = n_{r-1} = 0$ *and* $n_r \neq 0$ $(r \geqslant 2)$, *does not exist*.

Proof. Suppose the contrary, that is, that such graph G^* does exist. A vertex u of degree r is joined with all vertices $w_1, w_2, \ldots, w_r$ of maximum degree $n-1$. The graph G^* except vertices $u, w_1, w_2, \ldots, w_r$ contains still $n-r-1$ vertices. These $n-r-1$ vertices themselves do not form the complete graph. If they do form the complete graph, then the number of edges in G^* would be

$$m = \binom{n-r-1}{2} + r(n-r) + \binom{r}{2} = \frac{n^2-3n+2}{2} + r.$$

In this case G^* would have r edges more, contrary to our supposition ($m \leqslant (n^2 - 3n+2)/2$). It means that we can introduce at least $r-1$ edges between these $n-r-1$ vertices. Denote by G' a graph obtained from G^* when we delete $r-1$ edges between vertex u and vertices $w_2, w_3, \dots, w_r$ and introduce new $r-1$ edges between $r-1$ pairs of vertices: v_1 (degree j_1) and v_1' (degree j_1'), v_2 (j_2) and v_2' (j_2'),…,v_{r-1} (j_{r-1}) and v_{r-1}' (j_{r-1}'). Then

$$\begin{aligned} {}^0\chi(G') - {}^0\chi(G^*) &= \frac{1}{\sqrt{1}} - \frac{1}{\sqrt{r}} + \frac{r-1}{\sqrt{n-2}} - \frac{r-1}{\sqrt{n-1}} + \frac{1}{\sqrt{j_1+1}} - \frac{1}{\sqrt{j_1}} \\ &\quad + \frac{1}{\sqrt{j_1'+1}} - \frac{1}{\sqrt{j_1'}} + \frac{1}{\sqrt{j_2+1}} - \frac{1}{\sqrt{j_2}} + \frac{1}{\sqrt{j_2'+1}} - \frac{1}{\sqrt{j_2'}} + \cdots \\ &\quad + \frac{1}{\sqrt{j_{r-1}+1}} - \frac{1}{\sqrt{j_{r-1}}} + \frac{1}{\sqrt{j_{r-1}'+1}} - \frac{1}{\sqrt{j_{r-1}'}} \\ &> 1 - \frac{1}{\sqrt{r}} + 2(r-1)\left[\frac{1}{\sqrt{r+1}} - \frac{1}{\sqrt{r}}\right] \end{aligned}$$

because $1/\sqrt{j+1} - 1/\sqrt{j}$ is increasing function. Now we will prove that: $1 - 1/\sqrt{r} + 2(r-1)[1/\sqrt{r+1} - 1/\sqrt{r}] > 0$ for $r \geqslant 2$.

$$\begin{aligned} 1 - \frac{1}{\sqrt{r}} + 2(r-1)\left[\frac{1}{\sqrt{r+1}} - \frac{1}{\sqrt{r}}\right] &= \frac{r-1}{\sqrt{r}[\sqrt{r}+1]} - \frac{2(r-1)}{\sqrt{r}\sqrt{r+1}[\sqrt{r}+\sqrt{r+1}]} \\ &= \frac{r-1}{\sqrt{r}}\left\{\frac{1}{\sqrt{r}+1} - \frac{2}{\sqrt{r+1}[\sqrt{r}+\sqrt{r+1}]}\right\} > 0 \end{aligned}$$

because $\sqrt{r+1}(\sqrt{r+1}+\sqrt{r}) > 2\sqrt{r}+2$, namely $\sqrt{r(r+1)} > 2\sqrt{r}+1-r$ for $r \geqslant 2$. □

Finally, after considering all cases we proved the theorem. The extremal graph in the theorem is unique because inequality (8) is strict for $j \neq 0$.

Acknowledgements

I wish to thank Professor Pierre Hansen for his helpful advices.

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