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SOLUTION TO THE MINIMUM HARMONIC INDEX OF GRAPHS WITH GIVEN MINIMUM DEGREE

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ABSTRACT. The harmonic index of a graph G is defined as $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$, where $d(u)$ denotes the degree of a vertex u in G . Let $\mathcal{G}(n, k)$ be the set of simple n -vertex graphs with minimum degree at least k . In this work we consider the problem of determining the minimum value of the harmonic index and the corresponding extremal graphs among $\mathcal{G}(n, k)$. We solve the problem for each integer $k(1 \leq k \leq n/2)$ and show the corresponding extremal graph is the complete split graph $K_{k, n-k}^*$. This result together with our previous result which solve the problem for each integer $k(n/2 \leq k \leq n-1)$ give a complete solution of the problem.

1. Introduction

All graphs considered in the following will be simple. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The harmonic index $H(G)$ a graph G is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$

It has been found that the harmonic index correlate well with the Randić index [4, 5] and the π -electronic energy of benzenoid hydrocarbons [6]. To our best knowledge, this index first appear in [1], in which Favaron et al. considered the relation between harmonic index and the eigenvalues of graphs.

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Let $\mathcal{G}(n, k)$ be the set of n -vertex graphs with minimum degree at least k . In this work we consider the problem of determining the minimum value of the harmonic index and the corresponding extremal graphs among $\mathcal{G}(n, k)$. Zhong [8, 9] solved the problem for the case of $k = 1$ and gave some extremal results for trees and unicyclic graphs. Wu et al. [7] solved the result for the case of $k = 2$. Recently Liu [2], one of the authors, solved this problem for the cases of each integer $k(n/2 \leq k \leq n - 1)$. Thus, it is still an open problem for the cases of $k(3 \leq k < n/2)$. In this work, we solve this problem for each integer $k(1 \leq k < n/2)$ using a nonlinear programming model. Thus the problem of determining the minimum value of the harmonic index among $\mathcal{G}(n, k)$ is solved completely.

2. A nonlinear programming model for the harmonic index

We give a nonlinear programming model for the harmonic index in this section. We will see this model play a significant role in the proof of our main result.

Let G be a graphs of $\mathcal{G}(n, k)$. Denote by $x_{i,j}$ ($x_{i,j} \geq 0$), the number of edges joining the vertices of degrees i and j . Denote by n_i the number of vertices of degree of i . Then

$$(2.1) \quad H(G) = \sum_{k \leq i < j \leq n-1} \frac{2}{i+j} x_{i,j}$$

$$(2.2) \quad n_k + n_{k+1} + \cdots + n_{n-1} = n.$$

By counting the edges that incident to a vertex of degree i , $i = k, \dots, n - 1$, one obtains

$$(2.3) \quad \sum_{\substack{j=k \\ j \neq i}}^{n-1} x_{i,j} + 2x_{i,i} = in_i, \text{ i.e. } n_i = \frac{1}{i} \left(\sum_{\substack{j=k \\ j \neq i}}^{n-1} x_{i,j} + 2x_{i,i} \right).$$

Substituting Eq.(2.3) back into Eq.(2.2) and performing appropriate rearrangements, we get

$$(2.4) \quad \sum_{k \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} \right) x_{i,j} + 2 \sum_{i=k}^{n-1} \frac{x_{i,i}}{i} = n.$$

Now, rewriting Eq.(2.1) as

$$(2.5) \quad H(G) = \sum_{k \leq i < j \leq n-1} \frac{2}{i+j} x_{i,j} + \sum_{i=k}^{n-1} \frac{x_{i,i}}{i}$$

and combining Eq.(2.4) and Eq.(2.5) so as to eliminate the term $\sum(x_{ii}/i)$, we arrive at

$$n - 2H(G) = \sum_{k \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} = \sum_{k \leq i < j \leq n-1} \frac{(i-j)^2}{ij(i+j)} x_{i,j}$$

i.e.,

$$(2.6) \quad H(G) = \frac{n}{2} - \frac{1}{2} \sum_{k \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j}$$

$$(2.7) \quad = \frac{n}{2} - \frac{1}{2} \sum_{k \leq i < j \leq n-1} \frac{(i-j)^2}{ij(i+j)} x_{i,j}$$

Remark 2.1. From (2.7), we see that $H(G) \leq \frac{n}{2}$ for any n -vertex graph G and the equality holds if and only if G is regular. It is the reason why the problem of determining the maximum value of the harmonic index among $\mathcal{G}(n, k)$ is trivial.

We will give some linear equalities and nonlinear inequalities which must be satisfied in any above mentioned graph. By Eq. (2.6), the mathematical description of the problem (P) is

$$\min H = \frac{n}{2} - \frac{1}{2} \sum_{k \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j}$$

subject to

$$(2.8) \quad \sum_{\substack{j=k \\ j \neq i}}^{n-1} x_{i,j} + 2x_{i,i} = in_i \text{ for } k \leq i \leq n-1;$$

$$(2.9) \quad n_k + n_{k+1} + \dots + n_{n-1} = n;$$

$$(2.10) \quad x_{ij} \leq n_i n_j \text{ for } k \leq i < j \leq n-1;$$

$$(2.11) \quad x_{i,i} \leq \binom{n_i}{2} \text{ for } k \leq i \leq n-1;$$

$$(2.12) \quad x_{i,j}, n_i \in \mathbb{N}, k \leq i \leq j \leq n-1.$$

We can see the problem (P) together with (2.8)–(2.12) define a nonlinearly constrained optimization problem.

Thereafter the problem of minimization of H becomes the problem of maximization of

$$\gamma = \sum_{k \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{ij},$$

subject to (2.8)–(2.12).

Denote by $w(i, j) := \frac{1}{i} + \frac{1}{j} - \frac{4}{i+j}$ for simplicity. Note that $w(i, i) = 0$ for every positive integer i . Now we consider i and j as continuous variables and therefore we can take the partial derivative with respect to i and j , respectively. Then $\frac{\partial w(i,j)}{\partial i} = -\frac{1}{i^2} + \frac{4}{(i+j)^2} = \frac{(3i+j)(i-j)}{i^2(i+j)^2} < 0$ and $\frac{\partial w(i,j)}{\partial j} = -\frac{1}{j^2} + \frac{4}{(i+j)^2} = \frac{(i+3j)(j-i)}{j^2(i+j)^2} > 0$ for $i < j$. Thus, $w(i, j)$ is decreasing in i and increasing in j for $k \leq j < j \leq n-1$. We will use this property of $w(i, j)$ through the paper.

3. Main results

In this section, we will prove our main result using the nonlinear programming model mentioned above. Let $K_{k,n-k}^*$ be a complete split graph which is arised from a complete bipartite graph $K_{k,n-k}$ by joining each pair of vertices in the partite of k vertices.

Theorem 3.1. *Let G be a graph of $\mathcal{G}(n, k)$ for $1 \leq k < n/2$. Then*

$$H(G) \geq \frac{n}{2} - \frac{k(n-k)}{2} \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1} \right),$$

where equality holds if and only if $G \cong K_{k,n-k}^*$.

Proof. Let m be the index such that $n_m + n_{m+1} + \dots + n_{n-1} \geq k$ and $n_{m+1} + n_{m+2} + \dots + n_{n-1} < k$. We distinguish two subcases: (a) for such m holds $n_m + n_{m+1} + \dots + n_{n-1} = k$, and (b) $n_m + n_{m+1} + \dots + n_{n-1} > k$.

Subcase (a). $n_m + n_{m+1} + \dots + n_{n-1} = k$. We have:

$$\begin{aligned} \max \gamma &= \sum_{k \leq i < j \leq n-1} w(i, j)x_{i,j} \\ &= \sum_{i=k}^{m-1} \sum_{j=i+1}^{n-1} w(i, j)x_{i,j} + \sum_{m \leq i < j \leq n-1} w(i, j)x_{i,j}. \end{aligned}$$

We give the maximum possible values of $\sum_{j=i+1}^{n-1} w(i, j)x_{i,j}$ for $k \leq i \leq m-1$. Since $n_m + n_{m+1} + \dots + n_{n-1} = k$ and $\sum_{j=i+1}^{n-1} x_{i,j} \leq in_i$, first we join a vertex of degree i to all k vertices of degrees $n-1, \dots, m$ and last $i-k$ edges joining to $i-k$ vertices of degree $m-1$. Thus, holds:

$$\sum_{j=i+1}^{n-1} w(i, j)x_{i,j} \leq n_i \left(\sum_{j=m}^{n-1} w(i, j)n_j + w(i, m-1)(i-k) \right).$$

Therefore,

$$\max \gamma \leq \sum_{i=k}^{m-1} n_i \left(\sum_{j=m}^{n-1} w(i, j)n_j + w(i, m-1)(i-k) \right) + \sum_{m \leq i < j \leq n-1} w(i, j)x_{i,j}.$$

Denote $g(i) = \sum_{j=m}^{n-1} w(i, j)n_j + w(i, m-1)(i-k)$ and $f(x) = x(\frac{1}{x} + \frac{1}{y} - \frac{4}{x+y})$ for $0 < x < y$, then $f'(x) = \frac{1}{y} - \frac{4y}{(x+y)^2} < 0$. We have

$$k \cdot w(k, j) \geq i \cdot w(i, j), \text{ for } k \leq i \leq m-1, m \leq j \leq n-1.$$

Therefore,

$$\begin{aligned}
 g(i) &\leq \frac{k}{i} \left(\sum_{j=m}^{n-1} w(k, j)n_j + w(k, m-1)(i-k) \right) \\
 &= \sum_{j=m}^{n-1} w(k, j)n_j + \frac{i-k}{i} \left(w(k, m-1)k - \sum_{j=m}^{n-1} w(k, j)n_j \right) \\
 &\leq \sum_{j=m}^{n-1} w(k, j)n_j,
 \end{aligned}$$

because $\sum_{j=m}^{n-k} n_j = k$ and $w(k, m-1) < w(k, j)$ for $m \leq j \leq n-1$. Since $\sum_{j=k}^{m-1} n_j = n-k$, we have

$$\begin{aligned}
 \sum_{i=k}^{m-1} g(i)n_i &\leq \sum_{i=k}^{m-1} n_i \left(\sum_{j=m}^{n-1} w(k, j)n_j \right) \\
 &= (n-k) \sum_{j=m}^{n-1} w(k, j)n_j \\
 &= w(k, n-1)(n-k)n_{n-1} + \sum_{j=m}^{n-2} w(k, j)(n-k)n_j \\
 &= w(k, n-1)(n-k) \left(k - \sum_{j=m}^{n-2} n_j \right) + \sum_{j=m}^{n-2} w(k, j)(n-k)n_j \\
 &= w(k, n-1)(n-k)k + \sum_{j=m}^{n-2} \left(w(k, j) - w(k, n-1) \right) (n-k)n_j.
 \end{aligned}$$

Since $x_{i,j} \leq n_i n_j$ for $m \leq i < j \leq n-1$ and $n_{n-1} = k - \sum_{j=m}^{n-2} n_j$, we have:

$$\begin{aligned}
 \sum_{m \leq i < j \leq n-1} w(i, j)x_{i,j} &\leq \sum_{m \leq i < j \leq n-1} w(i, j)n_i n_j = \sum_{i=m}^{n-2} w(i, n-1)n_i n_{n-1} + \sum_{m \leq i < j \leq n-2} w(i, j)n_i n_j \\
 &= \sum_{i=m}^{n-2} w(i, n-1)n_i \left(k - \sum_{j=m}^{n-2} n_j \right) + \sum_{m \leq i < j \leq n-2} w(i, j)n_i n_j \\
 &= k \sum_{i=m}^{n-2} w(i, n-1)n_i - \sum_{i=m}^{n-2} \sum_{j=m}^{n-2} w(i, n-1)n_i n_j + \sum_{m \leq i < j \leq n-2} w(i, j)n_i n_j \\
 &= k \sum_{i=m}^{n-2} w(i, n-1)n_i - \sum_{i=m}^{n-2} w(i, n-1)n_i^2 - \sum_{m \leq i < j \leq n-2} \left(w(i, n-1) + w(j, n-1) \right) n_i n_j + \sum_{m \leq i < j \leq n-2} w(i, j)n_i n_j \\
 &= k \sum_{i=m}^{n-2} w(i, n-1)n_i - \sum_{i=m}^{n-2} w(i, n-1)n_i^2 - \sum_{m \leq i < j \leq n-2} \left(w(i, n-1) + w(j, n-1) - w(i, j) \right) n_i n_j
 \end{aligned}$$

Thus

$$\begin{aligned}
 \gamma &\leq w(k, n-1)(n-k)k + \sum_{j=m}^{n-2} \left((w(k, j) - w(k, n-1))(n-k) + w(j, n-1)k \right) n_j - \sum_{j=m}^{n-2} w(j, n-1)n_j^2 \\
 &\quad - \sum_{m \leq i < j \leq n-2} \left(w(i, n-1) + w(j, n-1) - w(i, j) \right) n_i n_j \\
 &\leq w(k, n-1)(n-k)k + \sum_{j=m}^{n-2} \left(w(k, j) - w(k, n-1) + w(j, n-1) \right) (n-k)n_j \\
 &\quad - \sum_{m \leq i < j \leq n-2} \left(w(i, n-1) + w(j, n-1) - w(i, j) \right) n_i n_j \\
 &\leq w(k, n-1)(n-k)k,
 \end{aligned}$$

where the second inequality holds because $k \leq \frac{n}{2} \leq n-k$ and $w(j, n-1) > 0$ for $m \leq j \leq n-2$. The last inequality holds because $h_1(j) = w(k, j) - w(k, n-1) + w(j, n-1) = \frac{2}{j} - \frac{4}{k+j} + \frac{4}{k+n-1} - \frac{4}{j+n-1} = \frac{2(k-j)}{j(k+j)} + \frac{4(j-k)}{(j+n-1)(k+n-1)} = 2(j-k) \left(\frac{2}{(j+n-1)(k+n-1)} - \frac{1}{j(k+j)} \right) = \frac{2(j-k)}{j(k+j)(j+n-1)(k+n-1)} \left(k(j-n+1) + (j^2 - j(n-1)) + (j^2 - (n-1)^2) \right) < 0$.

Denote $h_2(i, j) = w(i, n-1) + w(j, n-1) - w(i, j) = \frac{2}{n-1} + \frac{4}{i+j} - \frac{4}{i+n-1} - \frac{4}{j+n-1}$. We consider i and j as continuous variables, then $\frac{\partial h_2(i, j)}{\partial i} = -\frac{4}{(i+j)^2} + \frac{4}{(i+n-1)^2} < 0$ and $\frac{\partial h_2(i, j)}{\partial j} = -\frac{4}{(i+j)^2} + \frac{4}{(j+n-1)^2} < 0$, thus $h_2(i, j) > h_2(n-1, n-1) = 0$. Equality holds when $n_j = 0$ for $k+1 \leq j \leq n-2$, $n_k = n-k$, $n_{n-1} = k$, $x_{k, n-1} = (n-k)k$, $x_{n-1, n-1} = \binom{k}{2}$, and all other $x_{i, j}$ are equal to zero. Thus, the graph for which the harmonic index attains its minimum value is $K_{k, n-k}^*$.

Subcase (b). We put $n_m = n_{m'} + n_{m''}$, such that $n_{m''} + n_{m+1} + \dots + n_{n-1} = k$. Then $n_k + \dots + n_{m-1} + n_{m'} = n-k$. We will color the vertices of degree m with red and white, such that the number of red vertices is $n_{m''}$. Denote by $x_{i, m'}$ ($x_{i, m''}$) for $i \neq m$, the number of edges between vertices of degree i and the white (red) vertices of degree m , by $x_{m', m'}$ ($x_{m'', m''}$) the number of edges between white (red) vertices of degree m , and by $x_{m', m''}$ the number of edges between white and red vertices of degree m . Then $x_{i, m} = x_{i, m'} + x_{i, m''}$ for $i \neq m$, and $x_{m, m} = x_{m', m'} + x_{m', m''} + x_{m'', m''}$. We will replace system (2.8) by:

$$\begin{aligned}
 \sum_{k \leq j \leq n-1, j \neq i} x_{i, j} + 2x_{i, i} &= in_i, \text{ for } k \leq i \leq n-1, i \neq m, \\
 \sum_{k \leq j \leq n-1, i \neq m} x_{i, m'} + x_{m', m''} + 2x_{m', m'} &= mn_{m'}, \\
 \sum_{k \leq j \leq n-1, i \neq m} x_{i, m''} + x_{m', m''} + 2x_{m'', m''} &= mn_{m''}.
 \end{aligned}$$

We will proceed similarly as in the Subcase (a) and we omit the rest of the proof. □

An edge x_1x_2 is called *local maximum* if its weight $\frac{2}{d(x_1)+d(x_2)}$ is maximum in its neighborhood, i.e., $\frac{2}{d(x_1)+d(x_2)} \geq \frac{2}{d(x_i)+d(u)}$ for any edge x_iu for $i = 1, 2$.

Lemma 3.2. *Let x_1x_2 be a local maximum edge in graph G , then*

$$H(G) - H(G - x_1x_2) > 0.$$

Proof. We have

$$\begin{aligned} H(G) - H(G - x_1x_2) &= \frac{2}{d(x_1) + d(x_2)} + \sum_{u \in N(x_1) \setminus \{x_2\}} \left(\frac{2}{d(x_1) + d(u)} - \frac{2}{d(x_1) + d(u) - 1} \right) \\ &+ \sum_{v \in N(x_2) \setminus \{x_1\}} \left(\frac{2}{d(x_2) + d(v)} - \frac{2}{d(x_2) + d(v) - 1} \right) \\ &\geq \frac{2}{d(x_1) + d(x_2)} + (d(x_1) - 1) \left(\frac{2}{d(x_1) + d(x_2)} - \frac{2}{d(x_1) + d(x_2) - 1} \right) \\ &+ (d(x_1) - 1) \left(\frac{2}{d(x_1) + d(x_2)} - \frac{2}{d(x_1) + d(x_2) - 1} \right) \\ &= \frac{2}{(d(x_1) + d(x_2) - 1)(d(x_1) + d(x_2))} > 0, \end{aligned}$$

where $N(x_i)$ denotes the vertex set adjoining to x_i for $i = 1, 2$. □

For an edge x_1x_2 associates with a leaf, i.e. a vertex with degree one, we can see that it is a local maximum edge. Thus by Lemma 3.2 we have

Corollary 3.3. *If x_1x_2 is an edge in graph G such that x_1 is a leaf, then*

$$H(G) - H(G - x_1x_2) > 0.$$

For a graph $G \in \mathcal{G}(n, k)$. If $\delta(G) > k$, we always can find a local maximum edge uv and delete it. Then $\chi(G) \geq \chi(G - uv)$ and $H(G) > H(G - uv)$. This is the reason why the minimum degree of the extremal graphs which attaining the minimum value of the harmonic index among $\mathcal{G}(n, k)$ is k . Thus the problem of determining the minimum value of the harmonic index among $\mathcal{G}(n, k)$ is equal with the corresponding problem among n -vertex graphs with the minimum degree k .

4. Conclusion

We would like to conclude the problem of determining the minimum value of the harmonic index among $\mathcal{G}(n, k)$ with a complete answer. To do this, we need some notations. For two vertex disjoint graphs, G and F , let $G + F$ denote their join, i.e., the graph obtained by joining edges from every vertex of G to all vertices of F . One of the authors, Liu [2] proved that every graph with the minimum value of the harmonic index in $\mathcal{G}(n, k)$ for $k \geq n/2$ is a join between a regular graph and a complete graph. Let $\mathbf{F}(n, r)$ be the set of r -regular n -vertex graphs. We have $\mathbf{F}(n, r) \neq \emptyset$ if and only if $r \leq n - 1$ and nr is even (see for example [3]).

Theorem 4.1. [2] If G is an extremal graph attaining the minimum value of the harmonic index among $\mathcal{G}(n, k)$ for $k \geq n/2$, then G is a join between a regular graph and a complete graph, namely:

(1) If n is even, then: $H(G) = \frac{n}{2} - \frac{n^2}{8}w(k, n-1)$ and $G \cong F + K_{n/2}$, where $F \in \mathbf{F}(\frac{n}{2}, k - \frac{n}{2})$ for k even and $n \equiv 0 \pmod{4}$, k odd and $n \equiv 2 \pmod{4}$; $H(G) = \frac{n}{2} - \frac{n^2-4}{8}w(k, n-1)$ and $G \cong F + K_{\frac{n+2}{2}}$, where $F \in \mathbf{F}(\frac{n-2}{2}, k - \frac{n+2}{2})$ if $k \geq \frac{n+2}{2}$ for k even and $n \equiv 2 \pmod{4}$, or $H(G) = \frac{n}{2} - \frac{n^2-4}{8}w(k, n-1)$ and $G \cong F + K_{\frac{n-2}{2}}$, where $F \in \mathbf{F}(\frac{n+2}{2}, k - \frac{n-2}{2})$ for k even and $n \equiv 2 \pmod{4}$.

(2) If n is odd, then: $H(G) = \frac{n}{2} - \frac{n^2-1}{8}w(k, n-1)$ and $G \cong F + K_{\frac{n+1}{2}}$, where $F \in \mathbf{F}(\frac{n-1}{2}, k - \frac{n+1}{2})$ if $k \geq \frac{n+1}{2}$ for k even, k odd and $n \equiv 1 \pmod{4}$, or $H(G) = \frac{n}{2} - \frac{n^2-1}{8}w(k, n-1)$ and $G \cong F + K_{\frac{n-1}{2}}$, where $F \in \mathbf{F}(\frac{n+1}{2}, k - \frac{n-1}{2})$ for k even, k odd and $n \equiv 3 \pmod{4}$.

In short, the above theorem states that the extremal graph attaining the minimum value of the harmonic index among $\mathcal{G}(n, k)$ ($k \geq n/2$) has only two degrees, i.e., degree k and degree $n-1$, and n_k is as close to $n/2$ as possible. Therefore we conclude the paper with the following simple one. Reminding that n_k is the number of vertices of degree k .

Theorem 4.2. The extremal graph attaining the minimum value of the harmonic index among $\mathcal{G}(n, k)$ has only two degrees, i.e., degree k and degree $n-1$, and $n_k = n-k$ for $1 \leq k < n/2$ and n_k it is as close to $n/2$ as possible for $n/2 \leq k \leq n-1$.

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