



On a Conjecture of the Harmonic Index and the Minimum Degree of Graphs

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Abstract. The harmonic index of a graph G is defined as the sum of the weights $\frac{2}{d(u)+d(v)}$ of all edges uv of G , where $d(u)$ denotes the degree of the vertex u in G . Cheng and Wang [4] proposed a conjecture: For all connected graphs G with $n \geq 4$ vertices and minimum degree $\delta(G) \geq k$, where $1 \leq k \leq \lfloor \frac{n}{2} \rfloor + 1$, then $H(G) \geq H(K_{k,n-k}^*)$ with equality if and only if $G \cong K_{k,n-k}^*$. $K_{k,n-k}^*$ is a complete split graph which has only two degrees, i.e. degree k and degree $n - 1$, and the number of vertices of degree k is $n - k$, while the number of vertices of degree $n - 1$ is k . In this work, we prove that this conjecture is true when $k \leq \frac{n}{2}$, and give a counterexample to show that the conjecture is not correct when $k = \lfloor \frac{n}{2} \rfloor + 1$, n is even, that is $k = \frac{n}{2} + 1$.

1. Introduction

Throughout this paper we consider only simple connected graphs. Such a graph will be denoted by $G = (V(G), E(G))$, where $V(G)$ and $E(G)$ are the vertex set and edge set of G , respectively. For a vertex v of a graph G , we denote the degree of v by $d_G(v)$ ($d(v)$ for short). The minimum degree of G is denoted by $\delta(G)$. We use $G - uv$ to denote the graph that arises from G by deleting the edge $uv \in E(G)$. Let $G(n, k)$ be the set of connected simple graphs of order n with minimum degree k . We use $K_{k,n-k}^*$ to denote the graph that arises from the complete bipartite graph $K_{k,n-k}$ by joining every pair of vertices in the partite set with k vertices by a new edge. Our other notations are standard and taken mainly from [2].

The Randić index $R(G)$, proposed by Randić [11] in 1975, is defined as the sum of the weights $\frac{1}{\sqrt{d(u)d(v)}}$ over all edges uv of G , that is,

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

The Randić index is one of the most successful molecular descriptors in structure-property and structure-activity relationship studies. Mathematical properties of this descriptor have been studied extensively (see [7-9] and the references cited therein).

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Constraints (1) – (5) define a nonlinearly optimization problem.

If the first equality from (1) divide by k , second by $k + 1$, third by $k + 2$ and so on, the last by $n - 1$ and sum them all, we get

$$\sum_{k \leq i \leq j \leq n-1} \left(\frac{1}{i} + \frac{1}{j}\right)x_{i,j} = n_k + n_{k+1} + n_{k+2} + \dots + n_{n-1} = n$$

because of (2). Then

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

Define

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

Henceforth we will consider the problem of maximizing γ instead of minimizing $H(G)$.

3. Main result

Theorem 3.1. Let $G \in G(n, k)$, where $n \geq 4, 1 \leq k \leq \frac{n}{2}$. Then $H(G) \geq H(K_{k,n-k}^*)$ with equality if and only if $G \cong K_{k,n-k}^*$.

Proof. Since the minimum degree of G is k , it is obvious that $n_{n-1} \leq k$. Let m be the index such that $n_m + n_{m+1} + \dots + n_{n-2} + n_{n-1} \geq k$ and $n_{m+1} + \dots + n_{n-2} + n_{n-1} < k$. We distinguish two cases: (1) $n_m + \dots + n_{n-2} + n_{n-1} = k$, (2) $n_m + \dots + n_{n-2} + n_{n-1} > k$.

Case 1. $n_m + \dots + n_{n-2} + n_{n-1} = k$.

Note that

$$\begin{aligned} \gamma &= \sum_{k \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j}\right)x_{i,j} = \sum_{j=k+1}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j}\right)x_{k,j} + \sum_{j=k+2}^{n-1} \left(\frac{1}{k+1} + \frac{1}{j} - \frac{4}{k+1+j}\right)x_{k+1,j} + \dots \\ &\quad + \sum_{j=m}^{n-1} \left(\frac{1}{m-1} + \frac{1}{j} - \frac{4}{m-1+j}\right)x_{m-1,j} + \sum_{m \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j}\right)x_{i,j}. \end{aligned}$$

Weights of all edges which join vertices of degree i , with vertices of degree $j, i + 1 \leq j \leq n - 1$ are represented by $\sum_{j=i+1}^{n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j}\right)x_{i,j}$. We give the maximum possible weights to these edges. Since $n_m + \dots + n_{n-2} + n_{n-1} = k$ 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 $n - 1, \dots, m$ (maximum weights) and with $i - k$ vertices of other degrees $j, i + 1 \leq j \leq m - 1$. Furthermore, $h(x, y) = \frac{1}{x} + \frac{1}{y} - \frac{4}{x+y}$ is increasing for y , where $k \leq x < y \leq m - 1$ (since $\frac{\partial h(x,y)}{\partial y} = \frac{(y-x)(3y+x)}{y^2(x+y)^2} > 0$ for $k \leq x < y \leq m - 1$). We will

maximize the weights of these last $i - k$ edges joining a vertex of degree i to $i - k$ vertices of degree $m - 1$. Thus,

$$\begin{aligned} & \sum_{j=i+1}^{n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} \\ = & \sum_{j=m}^{n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} + \sum_{j=i+1}^{m-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} \\ \leq & \sum_{j=m}^{n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) n_i n_j + \left(\frac{1}{i} + \frac{1}{m-1} - \frac{4}{i+m-1} \right) (i-k) n_i \\ = & n_i \left(\sum_{j=m}^{n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) n_j + \left(\frac{1}{i} + \frac{1}{m-1} - \frac{4}{i+m-1} \right) (i-k) \right). \end{aligned}$$

Then

$$\begin{aligned} \gamma \leq & n_k \left(\left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1} \right) n_{n-1} + \left(\frac{1}{k} + \frac{1}{n-2} - \frac{4}{k+n-2} \right) n_{n-2} + \dots + \left(\frac{1}{k} + \frac{1}{m} - \frac{4}{k+m} \right) n_m \right) \\ & + n_{k+1} \left(\left(\frac{1}{k+1} + \frac{1}{n-1} - \frac{4}{k+n} \right) n_{n-1} + \left(\frac{1}{k+1} + \frac{1}{n-2} - \frac{4}{k+n-1} \right) n_{n-2} + \dots \right. \\ & \left. + \left(\frac{1}{k+1} + \frac{1}{m} - \frac{4}{k+1+m} \right) n_m + \left(\frac{1}{k+1} + \frac{1}{m-1} - \frac{4}{k+m} \right) \right) + \dots \\ & + n_{m-1} \left(\left(\frac{1}{m-1} + \frac{1}{n-1} - \frac{4}{m+n-2} \right) n_{n-1} + \left(\frac{1}{m-1} + \frac{1}{n-2} - \frac{4}{m+n-3} \right) n_{n-2} + \dots \right. \\ & \left. + \left(\frac{1}{m-1} + \frac{1}{m} - \frac{4}{2m-1} \right) n_m + \left(\frac{1}{m-1} + \frac{1}{m-1} - \frac{4}{2m-2} \right) (m-1-k) \right) \\ & + \sum_{m \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} \\ = & \sum_{k \leq i \leq m-1} f(i) n_i + \sum_{m \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} \\ = & \gamma_1 + \gamma_2 \end{aligned}$$

where $f(i) = \sum_{j=m}^{n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) n_j + \left(\frac{1}{i} + \frac{1}{m-1} - \frac{4}{i+m-1} \right) (i-k)$. Let $g(x) = x \left(\frac{1}{x} + \frac{1}{y} - \frac{4}{x+y} \right)$, where $0 < x < y$. Note that $g'(x) = \frac{(x-y)(x+3y)}{y(x+y)^2} < 0$ for $0 < x < y$, then $g(x)$ is monotonous decreasing for $0 < x < y$. Thus we have for $k+1 \leq i \leq m-1, m \leq j \leq n-1$:

$$k \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) \geq i \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right).$$

Therefore

$$\begin{aligned}
 f(i) &\leq \frac{k}{i} \left(\sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) n_j + \left(\frac{1}{k} + \frac{1}{m-1} - \frac{4}{k+m-1} \right) (i-k) \right) \\
 &= \left(1 - \frac{i-k}{i} \right) \left(\sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) n_j \right) + \frac{k(i-k)}{i} \left(\frac{1}{k} + \frac{1}{m-1} - \frac{4}{k+m-1} \right) \\
 &= \sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) n_j + \frac{i-k}{i} \left(\left(\frac{1}{k} + \frac{1}{m-1} - \frac{4}{k+m-1} \right) k - \sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) n_j \right) \\
 &\leq \sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) n_j,
 \end{aligned}$$

because $\sum_{j=m}^{n-1} n_j = k$ and $m \leq j \leq n-1$. Since $n_k + \dots + n_{m-1} = n-k$, we have

$$\begin{aligned}
 \gamma_1 &= \sum_{k \leq i \leq m-1} f(i) n_i \leq \left(\sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) n_j \right) \sum_{i=k}^{m-1} n_i \\
 &= (n-k) \sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) n_j = \sum_{j=m}^{n-1} \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1} \right) (n-k) n_j \\
 &\quad - \sum_{j=m}^{n-2} \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1} \right) (n-k) n_j + \sum_{j=m}^{n-2} \left(\frac{1}{k} + \frac{1}{j} - \frac{4}{k+j} \right) (n-k) n_j \\
 &= \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1} \right) (n-k) k - \sum_{j=m}^{n-2} \left(\frac{1}{n-1} + \frac{4}{k+j} - \frac{4}{k+n-1} - \frac{1}{j} \right) (n-k) n_j.
 \end{aligned}$$

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

$$\begin{aligned}
 \gamma_2 &= \sum_{m \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} \leq \sum_{m \leq i < j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) n_i n_j \\
 &= \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1} \right) n_i \left(k - \sum_{j=m}^{n-2} n_j \right) + \sum_{m \leq i < j \leq n-2} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) n_i n_j \\
 &= k \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1} \right) n_i - \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1} \right) n_i^2 \\
 &\quad + \sum_{m \leq i < j \leq n-2} \left(\left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) - \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1} \right) - \left(\frac{1}{j} + \frac{1}{n-1} - \frac{4}{j+n-1} \right) \right) n_i n_j \\
 &= k \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1} \right) n_i - \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1} \right) n_i^2 \\
 &\quad - 2 \sum_{m \leq i < j \leq n-2} \left(\frac{2}{i+j} + \frac{1}{n-1} - \frac{2}{i+n-1} - \frac{2}{j+n-1} \right) n_i n_j.
 \end{aligned}$$

Thus,

$$\begin{aligned}
 \gamma \leq \gamma_1 + \gamma_2 &\leq \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1}\right)(n-k)k - \sum_{i=m}^{n-2} \left(\frac{1}{n-1} + \frac{4}{k+i} - \frac{4}{k+n-1} - \frac{1}{i}\right)(n-k)n_i \\
 &+ k \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1}\right)n_i - \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1}\right)n_i^2 \\
 &- 2 \sum_{m \leq i < j \leq n-2} \left(\frac{2}{i+j} + \frac{1}{n-1} - \frac{2}{i+n-1} - \frac{2}{j+n-1}\right)n_i n_j \\
 &= \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1}\right)(n-k)k - \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1}\right)n_i^2 \\
 &- 2 \sum_{m \leq i < j \leq n-2} \left(\frac{2}{i+j} + \frac{1}{n-1} - \frac{2}{i+n-1} - \frac{2}{j+n-1}\right)n_i n_j \\
 &+ \sum_{i=m}^{n-2} \left(\left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1}\right)k - \left(\frac{1}{n-1} + \frac{4}{k+i} - \frac{4}{k+n-1} - \frac{1}{i}\right)(n-k)\right)n_i \\
 &\leq \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1}\right)(n-k)k - \sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1}\right)n_i^2 \\
 &- 2 \sum_{m \leq i < j \leq n-2} \left(\frac{2}{i+j} + \frac{1}{n-1} - \frac{2}{i+n-1} - \frac{2}{j+n-1}\right)n_i n_j \\
 &+ (n-k) \sum_{i=m}^{n-2} \left(\left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1}\right) - \left(\frac{1}{n-1} + \frac{4}{k+i} - \frac{4}{k+n-1} - \frac{1}{i}\right)\right)n_i \\
 &= \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1}\right)(n-k)k - \left(\sum_{i=m}^{n-2} \left(\frac{1}{i} + \frac{1}{n-1} - \frac{4}{i+n-1}\right)n_i^2\right. \\
 &+ 2 \sum_{m \leq i < j \leq n-2} \frac{(n-j-1)(2(n-1)(n+j-1) - (i+j)(n+i-1))}{(i+j)(n-1)(n+i-1)(n+j-1)}n_i n_j \\
 &\left. - 2(n-k) \sum_{i=m}^{n-2} \frac{(i-k)((i+n-1)(k+n-1) - (i+i)(k+i))}{i(k+i)(i+n-1)(k+n-1)}n_i\right) \\
 &\leq \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1}\right)(n-k)k.
 \end{aligned}$$

The second inequality holds because $k \leq n-k$. So $H(G) = \frac{n}{2} - \frac{\gamma}{2} \geq \frac{n}{2} - \frac{1}{2} \left(\frac{1}{k} + \frac{1}{n-1} - \frac{4}{k+n-1}\right)(n-k)k = \frac{k(k-1)}{2(n-1)} + \frac{2k(n-k)}{k+n-1} = H(K_{k,n-k}^*)$. Equality holds when $n_i = 0$ for $k+1 \leq i \leq n-2$, $n_k = n-k$, $n_{n-1} = k$, $x_{k,n-1} = (n-k)k$, $x_{n-1,n-1} = \binom{k}{2}$, and all other $x_{i,j}$ are equal to zero. Thus, graphs for which the harmonic index attains its minimum value are $K_{k,n-k}^*$.

Case 2. $n_m + \dots + n_{n-2} + n_{n-1} > k$.

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 $x_{i,m'}$ (resp. $x_{i,m''}$) for $i \neq m$, the number of edges between vertices of degree i and the white (resp. red) vertices of degree m , by $x_{m',m'}$ (resp. $x_{m'',m''}$) the number of edges between white (resp. 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 $x_{m,m} = x_{m',m'} + x_{m'',m''}$. We will replace system (1) by:

$$\begin{aligned} x_{k,i} + \cdots + x_{i,m-1} + x_{i,m'} + x_{i,m''} + x_{i,m+1} + \cdots + x_{i,n-1} &= in_i, k \leq i \leq n-1, i \neq m, \\ x_{k,m'} + \cdots + x_{m-1,m'} + 2x_{m',m'} + x_{m',m''} + x_{m',m+1} + \cdots + x_{m',n-1} &= mn_{m'}, \\ x_{k,m''} + \cdots + x_{m-1,m''} + x_{m',m''} + 2x_{m'',m''} + x_{m'',m+1} + \cdots + x_{m'',n-1} &= mn_{m''}. \end{aligned} \quad (1')$$

We will proceed similarly as in the Case 1. The rest of the proof is omitted, because it is similar to the one of Case 1. \square

Remark When $k = \frac{n}{2} + 1$, $n \equiv 0 \pmod{4}$ and $n \geq 8$, we give a counterexample to show that the Conjecture 1.1 is not correct. Let G' be an n -vertex graph obtained from K_n by deleting the edges of an $(\frac{n}{2} - 2)$ -regular graph on $\frac{n}{2}$ vertices. Then $G' \in G(n, \frac{n}{2} + 1)$. By some elementary calculations, we have $H(K_{\frac{n}{2}+1, \frac{n}{2}-1}^*) = \frac{n^2+2n}{8(n-1)} + \frac{n^2-4}{3n}$, $H(G') = \frac{n^2-2n}{8(n-1)} + \frac{n}{2(n+2)} + \frac{n}{3}$. Thus, $H(K_{\frac{n}{2}+1, \frac{n}{2}-1}^*) - H(G') = \frac{(n-4)^2}{6n(n-1)(n+2)} > 0$ for $n \geq 8$. This implies $H(K_{\frac{n}{2}+1, \frac{n}{2}-1}^*) > H(G')$.

When $k = \lfloor \frac{n}{2} \rfloor + 1$, n is odd, that is $k = \frac{n+1}{2}$, the graph G_1 in [1] is a counterexample which can show that the Conjecture 1.1 is also not correct.

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