Some spectral bounds for the harmonic matrix

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Abstract

The aim of this note is to establish new spectral bounds for the harmonic matrix.

The Harary matrix of given a connected graph G of order n, say $RD(G)$, is an n-by-n symmetric matrix, such that

$$(RD(G))_{ij} = \begin{cases} \frac{1}{d_{ij}}, & \text{if } i < j, \\ 0, & \text{if } i = j, \end{cases}$$

where d_{ij} denotes the distance between the vertices i and j [10, 11]. This matrix (originally known as reciprocal distance matrix [11]) is particulary well-known in chemistry. This is mainly motivated by the importance of the influence of the neighbor atoms when compared with the more distance ones [5, 9, 1].

If we consider a path of order n, with the vertices labeled in the standard way, the Harary matrix, say $A_n = (a_{i,j})$, will be defined as

$$a_{i,j} = \begin{cases} \dfrac{1}{|i-j|}, & \text{if } i \neq j, \\ 0, & \text{otherwise,} \end{cases} \tag{0.1}$$

which we will call harmonic matrix. The reason to adopt this name is intimately related with the harmonic numbers [13]. The nth harmonic number

$$H_n = \sum_{k=1}^{n} \frac{1}{k}$$

arises from the truncation of the harmonic series. One of the most interesting analytical expression for these numbers is

$$H_n = \gamma + \Psi(n+1),$$

where γ is the Euler-Mascheroni constant and $\Psi(\cdot)$ is the digamma function. Clearly, we can extend this concept to

$$H_n^{(r)} = \sum_{k=1}^{n} \frac{1}{k^r},$$

which we may designate by rth harmonic number, where $H_n^{(1)} = H_n$.

The harmonic spectrum of A_n is

$$\mathrm{Spec}_H(A_n) = \{\sigma_1, \sigma_2, \ldots, \sigma_n\},$$

where $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_n$ are the eigenvalues of A_n, arranged in non-increasing order. Sometimes we use $\sigma \, (= \sigma_1)$ to denote the largest eigenvalue of A_n. For example, the 5×5 harmonic matrix is

$$A_5 = \begin{pmatrix} 0 & 1 & 1/2 & 1/3 & 1/4 \\ 1 & 0 & 1 & 1/2 & 1/3 \\ 1/2 & 1 & 0 & 1 & 1/2 \\ 1/3 & 1/2 & 1 & 0 & 1 \\ 1/4 & 1/3 & 1/2 & 1 & 0 \end{pmatrix}.$$

The eigenvalues of A_5 are:

$$2.61684, \; 0.303284, \; -0.560813, \; -1.05328, \; -1.30603 \,.$$

Another surprising application of the harmonic matrix is related to the study of the invertibility of the Foldy-Lax algebraic systems associated to both homogeneous and nonhomogeneous. The matrix commonly considered

(cf. e.g. [2, 3, 4]) is

$$B = \begin{pmatrix} \frac{1}{C_1} & \Phi_\kappa(z_1, z_2) & \Phi_\kappa(z_1, z_3) & \cdots & \Phi_\kappa(z_1, z_n) \\ \Phi_\kappa(z_1, z_2) & \frac{1}{C_2} & \Phi_\kappa(z_2, z_3) & \ddots & \vdots \\ \Phi_\kappa(z_1, z_3) & \Phi_\kappa(z_2, z_3) & \frac{1}{C_3} & \ddots & \Phi_\kappa(z_{n-2}, z_n) \\ \vdots & \ddots & \ddots & \ddots & \Phi_\kappa(z_{n-1}, z_n) \\ \Phi_\kappa(z_1, z_n) & \cdots & \Phi_\kappa(z_{n-2}, z_n) & \Phi_\kappa(z_{n-1}, z_n) & \frac{1}{C_n} \end{pmatrix},$$

$$(0.2)$$

where the fundamental solution, $\Phi(x, y)$, of the Helmholtz equation in $\mathbb{R}^3$ with the fixed wave number κ is given by

$$\Phi(x, y) = \frac{e^{i\kappa|x-y|}}{4\pi|x-y|}, \quad \text{for all } x, y \in \mathbb{R}^3,$$

and C_k's are coefficients based on surfaces area and impedance. There are some known sufficient conditions for the invertibility of B, but not necessary [2, 3, 4]. Inverting B in general seems a hard problem. So, we normally want find a way to compute the inverse of B as much generality as possible or eventually find necessary and sufficient conditions for its invertibility. If one considers the case where the distance between the centers of the consecutive scatterers is the same, i.e., distributing the scatterers in a uniform array, and the capacitances of the scatterers are also the same, i.e., the C_k's are equal, then B is symmetric Toeplitz matrix, but not circulant. These considerations lead us, for $\kappa = 0$, to the matrices of the form

$$A_{nr} = \begin{pmatrix} 0 & \frac{1}{r} & \frac{1}{2r} & \cdots & \frac{1}{(n-1)r} \\ \frac{1}{r} & 0 & \frac{1}{r} & \ddots & \vdots \\ \frac{1}{2r} & \frac{1}{r} & 0 & \ddots & \frac{1}{2r} \\ \vdots & \ddots & \ddots & \ddots & \frac{1}{r} \\ \frac{1}{(n-1)r} & \cdots & \frac{1}{2r} & \frac{1}{r} & 0 \end{pmatrix}, \quad (0.3)$$

Finally, for $r = 1$ we get the harmonic matrix (0.1).

Our aim is to establish several new results on the spectra of the harmonic matrices. It would be interesting to analyze in particular what happens in the case of the more general matrices (0.3).

1 Known bounds

In this section we present several known bounds applied to the harmonic matrix (0.1). The first theorem is a general result.

Lemma 1.1. *[8, Theorem 8.1.22] Let $A = (A_{i,j})$ be an $n \times n$ irreducible nonnegative matrix with spectral radius σ and let $R_i(A) = \sum_{j=1}^{n} a_{i,j}$ be the ith row sum of A. Then*

$$\min\{R_i(A) : 1 \leqslant i \leqslant n\} \leqslant \sigma \leqslant \max\{R_i(A) : 1 \leqslant i \leqslant n\}. \qquad (1.1)$$

Moreover, if the row sums of A are not all equal, then the both inequalities in (1.1) are strict.

For A_5, we have $2.08333 < \sigma < 3$.

From the bounds produced in [14] we have

$$\sigma \leqslant \frac{3n-4}{4}$$

if n is even, and

$$\sigma \leqslant \frac{n-2+\sqrt{4n^2-3}}{4}$$

otherwise. For the case of A_5, the bound is 3.21221. From the same reference, we have

$$\sigma \leqslant \frac{3n-6+\sqrt{17n^2+28n+4}}{8},$$

if n is even, and

$$\sigma \leqslant \frac{3n-5+\sqrt{17n^2+34n-15}}{8},$$

otherwise. For A_5, the bound is 4.2604.

The bounds found by Zhou and Trinajstić in [15] give us

$$\sqrt{\frac{\sum_{i=1}^{n} R_i^2}{n}} < \sigma < \max_i \sum_{j=1}^{n} h_{ij} \sqrt{\frac{R_j}{R_i}}.$$

In the current example we get $2.59754 < \sigma < 2.77698$. Another bound from these authors is $3 - \frac{4}{n} < \sigma$. Here, we have $2.2 < \sigma$.

The first author in [6] established the bound

$$\sigma \leqslant \frac{\sqrt{n^2+4n-8}}{2}.$$

For $n = 5$, we get $\sigma < 3.04138$.

2 New bounds

We now give an upper bound for the spectral radius of the harmonic matrix A_n.

Theorem 2.1. *For the harmonic matrix A_n, we have*

$$\sigma(A_n) < \begin{cases} \frac{n}{100} + 8.356 + \frac{2}{n} & \text{if } n \text{ is even,} \\[2mm] \frac{n}{100} + 8.366 & \text{if } n \text{ is odd.} \end{cases}$$

Proof. By Lemma 1.1, we have

$$\sigma(A_n) < \begin{cases} 2\left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{2}{n-2}\right) + \frac{2}{n} & \text{if } n \text{ is even,} \\[3mm] 2\left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{2}{n-1}\right) & \text{if } n \text{ is odd,} \end{cases}$$

that is

$$\sigma(A_n) < \begin{cases} 2\,H_{p-1} + \frac{1}{p} & \text{if } n = 2p, \\[3mm] 2\,H_p & \text{if } n = 2p+1. \end{cases} \tag{2.1}$$

One can easily get that

$$1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{100} < 5.18738\,.$$

Using the above result, we have

$$2\left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{2}{n-1}\right) < 2\left[\left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{100}\right) + \frac{1}{100} \times \left(\frac{n-1}{2} - 100\right)\right]$$

$$< \quad 2\left[5.188 + \frac{n-201}{200}\right]$$

$$= \quad \frac{n}{100} + 8.366.$$

Similarly,

$$2\left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{2}{n-1}\right) + \frac{2}{n} \quad < \quad \frac{n}{100} + 8.356 + \frac{2}{n}\,.$$

This completes the proof. □

We now give a lower bound on $\sigma(A_n)$.

Theorem 2.2. *Let A_n be an $n \times n$ matrix defined in* (0.1). *Then*

$$\sigma(A_n) \geqslant \sqrt{\frac{2}{n} \sum_{i=1}^{n-1} \frac{n-i}{i^2}}. \tag{2.2}$$

Proof. We have

$$\mathrm{tr}(A_n^2) = 2 \left[n - 1 + \frac{n-2}{2^2} + \frac{n-3}{3^2} + \cdots + \frac{2}{(n-2)^2} + \frac{1}{(n-1)^2} \right]$$

$$= 2\,n \left(1 + \frac{1}{2^2} + \frac{1}{3^2} + \cdots + \frac{1}{(n-1)^2} \right) - 2 \left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{(n-1)} \right)$$

$$= 2 \sum_{i=1}^{n-1} \frac{n-i}{i^2}.$$

Therefore we have

$$n\,\sigma^2(A_n) \geqslant \mathrm{tr}\left(A_n^2\right) = 2 \sum_{i=1}^{n-1} \frac{n-i}{i^2},$$

which gives the required result. $\qquad\square$

Lemma 2.3. *Let A_n be the harmonic matrix of order n. If Y is a subset of $\{2, 3, \ldots, n\}$, then*

$$\sum_{i \in Y} \sigma_i^2(A_N) \leqslant \frac{2(n-1)}{n} \sum_{i=1}^{n-1} \frac{n-i}{i^2}.$$

Proof. We have

$$\sum_{i \in Y} \sigma_i^2(A_n) \leqslant \sum_{i=1}^{n} \sigma_i^2(A_n) - \sigma_1^2(A_n). \tag{2.3}$$

Since

$$\sum_{i=1}^{n} \sigma_i^2(A_n) = \mathrm{tr}(A_n^2) = 2 \sum_{i=1}^{n-1} \frac{n-i}{i^2},$$

by Theorem 2.2 with (2.3), we get the required result. $\qquad\square$

Theorem 2.4. *Let A_n be the harmonic matrix of order n. If $\sigma_k(A_n) \leqslant 0$, for $2 \leqslant k \leqslant n$, then*

$$|\sigma_k(A_n)| \leqslant \sqrt{\frac{2(n-1)}{n(n-k+1)}} \sqrt{\sum_{i=1}^{n-1} \frac{n-i}{i^2}} \, .$$

Proof. Since $\sigma(A_n) \geqslant \sigma_2(A_n) \geqslant \cdots \geqslant \sigma_n(A_n)$, one can see easily that

$$(n-k+1)\,\sigma_k^2(A_n) \leqslant \sum_{i=k}^{n} \sigma_i^2(A_n) \leqslant \sum_{i=2}^{n} \sigma_i^2(A_n) \leqslant \frac{2(n-1)}{n} \sum_{i=1}^{n-1} \frac{n-i}{i^2} \, , \text{for } k \geqslant 2.$$

Hence the theorem follows. $\qquad\square$

Corollary 2.5. *Let A_n be the harmonic matrix of order n. Then*

$$|\sigma_n(A_n)| \leqslant \sqrt{\frac{2(n-1)}{n}} \cdot \sqrt{\sum_{i=1}^{n-1} \frac{n-i}{i^2}} \, .$$

Proof. By Theorem 2.4, we get the required result. $\qquad\square$

Gregory et al. [7, Theorem 2.1] obtained the spread of the spectrum of the adjacency matrix of graph G. Using the same technique, we give an upper bound for $\sigma - \sigma_n$. We omit its proof.

Theorem 2.6. *Let A_n be the harmonic matrix of order n and precisely k negative eigenvalues. Then*

$$\sigma - \sigma_n \leqslant \left(1 + \frac{1}{k}\right)\sigma + \sqrt{2\left(1 - \frac{1}{k}\right)\sum_{i=1}^{n-1}\frac{n-i}{i^2} - \left(1 - \frac{1}{k^2}\right)\sigma^2}. \qquad (2.4)$$

Notice that all our news bounds are significantly better and useful for larger orders n.

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