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Bounds on the Spectral Radius of the Line Distance Matrix *

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Abstract: The greatest eigenvalue of a line distance matrix D, denoted by $\lambda(D)$, is called the spectral radius of D. In this paper, we obtain some sharp upper and lower bounds for $\lambda(D)$.

1 Introduction

Let $\mathbf{t}= (t_1, t_2, ..., t_n)$, $t_1 < t_2 < ... < t_n$, $t_i \in \mathbb{R}$, be a given position vector (i.e., a list of points on the real line). *A line distance matrix* $D \in \mathbb{R}^{n\times n}$, associated with $\mathbf{t}$ is defined as $D = (d_{ij})$, where $d_{ij} = |t_i - t_j|$. The symbol $\lambda(D)$, called the *spectral radius* of D, is the largest eigenvalue of D. Throughout this paper, D is always defined as the line distance matrix of $\mathbf{t}$.

One of the main areas of Bioinformatics is the study of biological sequences. Recently, alternative routes for quantitative measure of the degree of similarity of DNA sequences were considered, which have also been extended to protein sequences. The novel methodology starts with a graphical representation of DNA, such as proposed by Nandy [1], which are subsequently numerically characterized by associating with the selected geometrical object that represents DNA, a matrix [2]. Another approach is to associate a matrix to a

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given sequence and study its properties instead [3]. Such a representation, based on the sequential labels of each of the four nucleotides A, T, G, and C separately for construction of matrix elements is given in [4]. A line distance matrix represents distance between points on the real line, therefore it gives a natural way of studying biological sequences. For more information on the application of line distance matrix to Biology and the recent results one can refer to [3,9] and the references cited therein.

Recently, it has been shown that a line distance matrix of size $n > 1$ has one positive and $n-1$ negative eigenvalues [3]. In this paper, some sharp upper and lower bounds for the spectral radius of a line distance matrix are obtained.

2 Main results

For the spectral radius of a non-negative matrix, it is well known that

Lemma 2.1 [5] *Let $M = (m_{ij})$ be an $n \times n$ irreducible non-negative matrix with spectral radius $\lambda(M)$, and let $R_i(M)$ be the i-th row sum of M, i.e., $R_i(M) = \sum_{j=1}^{n} m_{ij}$. Then,*

$$min\{R_i(M) : 1 \le i \le n\} \le \lambda(M) \le max\{R_i(M) : 1 \le i \le n\}. \tag{1}$$

Moreover, if the row sums of M are not all equal, then the both inequalities in (1) *are strict.*

In the following, let D_i denote the i-th row sum of D, i.e., $D_i = \sum_{j=1}^{n} d_{ij}$. Recall that D is the line distance matrix of $\mathbf{t}$, where $\mathbf{t}= (t_1, t_2, ..., t_n)$ and $t_1 < t_2 < ... < t_n$, it follows that

$$D_i = \begin{cases} t_{i+1} + \cdots + t_n - (n-2i+1)t_i - t_1 - \cdots - t_{i-1} & \text{if} \quad 1 \le i \le n-1 \\ (n-1)t_n - t_1 - \cdots - t_{n-1} & \text{if} \quad i = n \end{cases} \tag{2}$$

Theorem 2.1 *Let $\mathbf{t}= (t_1, t_2, ..., t_n)$, $t_1 < t_2 < ... < t_n$, D be the line distance matrix of $\mathbf{t}$, and D_i as denoted in equality* (2)*. If s is a real number, then*

$$min\{\sum_{j=1}^{n} d_{ij}(\frac{D_j}{D_i})^s : 1 \le i \le n\} \le \lambda(D) \le max\{\sum_{j=1}^{n} d_{ij}(\frac{D_j}{D_i})^s : 1 \le i \le n\}. \tag{3}$$

Equality on both sides of (3) *is attained if and only if $\sum_{j=1}^{n} d_{1j}(\frac{D_j}{D_1})^s = \sum_{j=1}^{n} d_{2j}(\frac{D_j}{D_2})^s = \cdots = \sum_{j=1}^{n} d_{nj}(\frac{D_j}{D_n})^s$.*

Proof. Let $B = diag(D_1^s, D_2^s, ..., D_n^s)$, i.e., the diagonal matrix with D_i^s as its i-th diagonal element and zero elsewhere. Denote by $B^{-1}DB = C = (c_{ij})$, then $c_{ij} = d_{ij}(\frac{D_j}{D_i})^s$. Since $t_1 < t_2 < ... < t_n$, D is a non-negative irreducible matrix. This implies that C is also a non-negative irreducible matrix. Note that $\lambda(D) = \lambda(B^{-1}DB)$, then Lemma 2.1 implies the inequalities (3), and the corresponding statements for equalities hold. ∎

Corollary 2.1 *Let* **t**$= (t_1, t_2, ..., t_n)$*,* $t_1 < t_2 < ... < t_n$*,* D *be the line distance matrix of* **t***, and* D_i *as denoted in equality* (2)*. If* k *is an integer, then*

$$min\{\sum_{j=1}^{n} d_{ij}(\frac{D_j}{D_i})^k : 1 \leq i \leq n\} \leq \lambda(D) \leq max\{\sum_{j=1}^{n} d_{ij}(\frac{D_j}{D_i})^k : 1 \leq i \leq n\}.$$

Equality on both sides is attained if and only if $\sum_{j=1}^{n} d_{1j}(\frac{D_j}{D_1})^k = \sum_{j=1}^{n} d_{2j}(\frac{D_j}{D_2})^k = \cdots = \sum_{j=1}^{n} d_{nj}(\frac{D_j}{D_n})^k$.

Theorem 2.2 *Let* **t**$= (t_1, t_2, ..., t_n)$*,* $t_1 < t_2 < ... < t_n$*. If* D *is the line distance matrix of* **t** *, then*

$$\frac{2}{n} \sum_{1 \leq i < j \leq n} (t_j - t_i) \leq \lambda(D) \leq max\{(n-1)t_n - \sum_{i=1}^{n-1} t_i, \sum_{i=2}^{n} t_i - (n-1)t_1\}. \tag{4}$$

Equality on both sides of (4) *is attained if and only if* $n = 2$*.*

Proof. Recall that the i-th row sum of D is equal to D_i, where D_i is denoted in equality (2). Clearly,

$$D_i - D_{i+1} = \begin{cases} (n-2i)(t_{i+1} - t_i) \geq 0 & \text{when} \quad 1 \leq i \leq \lfloor \frac{n}{2} \rfloor \\ (n-2i)(t_{i+1} - t_i) \leq 0 & \text{when} \quad \lceil \frac{n}{2} \rceil \leq i \leq n-1 \end{cases} \tag{5}$$

By Lemma 2.1 and equality (5) it follows that $\lambda(D) \leq max\{D_i : 1 \leq i \leq n\} = max\{D_1, D_n\}$. Thus, the upper bound of (4) follows. If $n = 2$, then $\lambda(D) = t_2 - t_1$, thus the equality holds. On the converse, if $n \geq 3$, then $D_1 > D_2$ by equality (5). By Lemma 2.1, the right inequality is strict. Thus, the right equality only holds for $n = 2$.

Let $x = \frac{1}{\sqrt{n}}(1, ..., 1)$ be a unit n-vector. Apply Raleigh principle to the line distance matrix D of **t**, we have

$$\lambda(D) \geq \frac{xDx^T}{xx^T} = \frac{1}{n} \sum_{i=1}^{n} D_i = \frac{2}{n} \sum_{1 \leq i < j \leq n} (t_j - t_i).$$

If the left equality holds, then x^T is the eigenvector corresponding to $\lambda(D)$, and hence $Dx^T = \lambda(D)x^T$. This implies that $D_i = \lambda(D)$ for all i. Thus, $n = 2$ by the above discussion. Conversely, if $n = 2$, then $\lambda(D) = t_2 - t_1$, thus the left equality also holds. ∎

Remark 1. Take $s = 0$ in Theorem 2.1 (and Corollary 2.1), we have

$$\lambda(D) \leq max\{\sum_{j=1}^{n} d_{ij} : 1 \leq i \leq n\} = max\{D_i : 1 \leq i \leq n\} = max\{D_1, D_n\}.$$

Thus, the upper bound of Theorem 2.2 is just a special case of Theorem 2.1 (and Corollary 2.1).

Theorem 2.3 *Let* $\mathbf{t}= (t_1, t_2, ..., t_n)$, $t_1 < t_2 < ... < t_n$, *and* D *be the line distance matrix of* $\mathbf{t}$. *Let* D_i *be denoted as equality* (2), *and* $T_i(s) = \sum_{j=1}^{n} d_{ij} D_j^s$, *where* s *is a real number. Then,*

$$\lambda(D) \geq \sqrt{\frac{T_1^2(s) + \cdots + T_n^2(s)}{D_1^{2s} + \cdots + D_n^{2s}}}.$$

Equality holds if and only if $\frac{T_i(s)}{D_i^s} = k$ *for* $1 \leq i \leq n$.

Proof. This proof follows ideas of Indulal, used for obtaining the lower bound for the spectral radius of the distance matrix pertaining to a graph [6]. Let $x = \frac{1}{\sqrt{D_1^{2s}+\cdots+D_n^{2s}}}(D_1^s, ..., D_n^s)$, then x is a unit positive n-vector. By Raleigh principle, we have

$$\lambda(D) = \sqrt{\lambda(D^2)} \geq \sqrt{\frac{xD^2x^T}{xx^T}} = \sqrt{xD^2x^T}.$$

On the other hand, since

$$xD^2x^T = xDDx^T = (Dx^T)^T Dx^T = \frac{T_1^2(s) + \cdots + T_n^2(s)}{D_1^{2s} + \cdots + D_n^{2s}},$$

the inequality holds. Now assume the equality holds, then x^T is the eigenvector corresponding to $\lambda(D)$, thus $\frac{T_i(s)}{D_i^s} = k = \lambda(D)$. Conversely, if $\frac{T_i(s)}{D_i^s} = k$, then $Dx^T = kx^T$. By the Perron-Frobenius Theorem, k is simple and the greatest eigenvalue of D. ∎

Set $s = 0$ in Theorem 2.3 and note that $T_i(0) = D_i$, we have

Corollary 2.2 *Let* $\mathbf{t}= (t_1, t_2, ..., t_n)$, $t_1 < t_2 < ... < t_n$, *and* D *be the line distance matrix of* $\mathbf{t}$. *Let* D_i *be denoted as in equality* (2), *then*

$$\lambda(D) \geq \sqrt{\frac{D_1^2 + \cdots + D_n^2}{n}}.$$

Equality holds if and only if $n = 2$.

Set $s = 1$ in Theorem 2.3, it follows that

Corollary 2.3 *Let* $\mathbf{t}=(t_1, t_2, ..., t_n)$, $t_1 < t_2 < ... < t_n$, *and* D *be the line distance matrix of* $\mathbf{t}$. *Let* D_i *be denoted as equality* (2), *and* $T_i = \sum_{j=1}^{n} d_{ij} D_j$. *Then,*

$$\lambda(D) \geq \sqrt{\frac{T_1^2 + \cdots + T_n^2}{D_1^2 + \cdots + D_n^2}}.$$

Equality holds if and only if $\frac{T_i}{D_i} = k$ *for* $1 \leq i \leq n$.

Lemma 2.2 $T_1 + \cdots + T_n = D_1^2 + \cdots + D_n^2$.

Proof. Recall that $D_i = \sum_{j=1}^{n} d_{ij}$ and $T_i = \sum_{j=1}^{n} d_{ij} D_j$, then

$$\begin{aligned} T_1 + \cdots + T_n &= [1, 1, ..., 1](D[D_1, D_2, ..., D_n]^T) \\ &= ([1, 1, ..., 1]D)[D_1, D_2, ..., D_n]^T \\ &= [D_1, D_2, ..., D_n][D_1, D_2, ..., D_n]^T \\ &= D_1^2 + \cdots + D_n^2. \end{aligned}$$

Thus, the equality holds. ∎

Theorem 2.4 *The lower bound for* $\lambda(D)$ *is improving from Theorem* 2.2 *to Corollary* 2.2, *and also improving from Corollaries* 2.2 *to* 2.3.

Proof. This proof is fully analogous to what Indulal has done in the case of the spectral radius of the distance matrix pertaining to a graph [6]. By Lemma 2.2 and Cauchy-Schwartz inequality, it follows that

$$\begin{aligned} \sqrt{\frac{T_1^2 + \cdots + T_n^2}{D_1^2 + \cdots + D_n^2}} &\geq \sqrt{\frac{(T_1 + \cdots + T_n)^2}{n(D_1^2 + \cdots + D_n^2)}} \\ &= \sqrt{\frac{(D_1^2 + \cdots + D_n^2)^2}{n(D_1^2 + \cdots + D_n^2)}} \\ &= \sqrt{\frac{D_1^2 + \cdots + D_n^2}{n}} \\ &\geq \sqrt{\frac{(D_1 + D_2 + \cdots + D_n)^2}{n^2}} \\ &= \frac{1}{n} \sum_{i=1}^{n} D_i = \frac{2}{n} \sum_{1 \leq i < j \leq n} (t_j - t_i). \end{aligned}$$

This completes the proof. ∎

Remark 2. By Theorem 2.2, it follows that

$$\lambda(D) \geq \frac{2}{n}\sum_{1\leq i<j\leq n}(t_j - t_i) = \frac{1}{n}\sum_{i=1}^{n} D_i \geq min\{D_i : 1 \leq i \leq n\} = min\{\sum_{j=1}^{n} d_{ij} : 1 \leq i \leq n\}.$$

Thus, the lower bound of Theorem 2.2 (and Corollaries 2.2–2.3 by Theorem 2.4) is better than lower bound of Theorem 2.1 for $s = 0$. But unfortunately, the lower bounds of Theorem 2.1 and Corollary 2.3 are incomparable. For example, take $\mathbf{t}= (1, 4, 7)$ and $s = 0.77$. By Theorem 2.1 and Corollary 2.3, we have

$$\begin{aligned}\lambda(D) &\geq min\{\sum_{j=1}^{3} d_{ij}(\frac{D_j}{D_i})^{0.77} : 1 \leq i \leq 3\}\\ &= 6 + 3 \times (2/3)^{0.77}\\ &> 8.195\\ &> \sqrt{\frac{72^2 + 54^2 + 72^2}{9^2 + 6^2 + 9^2}}\\ &= \sqrt{\frac{T_1^2 + T_2^2 + T_3^2}{D_1^2 + D_2^2 + D_3^2}}.\end{aligned}$$

Thus, the lower bound of Theorem 2.1 is finer than Corollary 2.3 in this case.

Remark 3. By Theorem 2.4 and Remark 2, the lower bounds of Corollary 2.2 and Theorem 2.1 are incomparable, and the lower bound of Theorem 2.1 is also incomparable with Theorem 2.2.

Lemma 2.3 [7] (Papendieck and Recht) *Let $q_1, q_2, ..., q_n$ be n positive numbers, then*

$$min\{\frac{p_i}{q_i} : 1 \leq i \leq n\} \leq \frac{\sum_{i=1}^{n} p_i}{\sum_{i=1}^{n} q_i} \leq max\{\frac{p_i}{q_i} : 1 \leq i \leq n\}$$

for any real number $p_1, p_2, ..., p_n$. Equality holds on either side if and only if all the ratios p_i/q_i are equal.

Remark 4. By Lemma 2.3, we can conclude that

$$\begin{aligned}\sqrt{\frac{T_1^2(s) + \cdots + T_n^2(s)}{D_1^{2s} + \cdots + D_n^{2s}}} &\geq \sqrt{min\{(\frac{T_i(s)}{D_i^s})^2 : 1 \leq i \leq n\}}\\ &= min\{\frac{T_i(s)}{D_i^s} : 1 \leq i \leq n\}\\ &= min\{\sum_{j=1}^{n} d_{ij}(\frac{D_j}{D_i})^s : 1 \leq i \leq n\}.\end{aligned}$$

Thus, the lower bound of Theorem 2.3 is always finer than Theorem 2.1.

Given two $n \times n$ matrixes $B = (b_{ij})$ and $C = (c_{ij})$, by $C \geq B$ we mean that $c_{ij} \geq b_{ij}$ for any i and j.

Lemma 2.4 [8] *Let $M = (m_{ij})$ be a non-negative irreducible matrix of order $n > 1$, and $B = (b_{ij})$ be a non-negative matrix of order n. If $M \geq B$, then $\lambda(M) \geq \lambda(B)$. Moreover, the equality holds if and only if $M = B$.*

Theorem 2.5 *Let* $\mathbf{t}= (t_1, t_2, ..., t_n)$, $t_1 < t_2 < ... < t_n$, *and* $\mathbf{t'}= (t'_1, t'_2, ..., t'_n)$, $t'_1 < t'_2 < ... < t'_n$. *Let D and D' be the line distance matrices of* $\mathbf{t}$ *and* $\mathbf{t'}$, *respectively. If $t_1 > t'_1$ and $t_i = t'_i$ for $2 \leq i \leq n$, or $t_n < t'_n$ and $t_i = t'_i$ for $1 \leq i \leq n-1$, then $\lambda(D) < \lambda(D')$.*

Proof. We only consider the case of $t_1 > t'_1$ and $t_i = t'_i$ for $2 \leq i \leq n$, because another case can be considered similarly. Suppose $D = (d_{ij})$ and $D' = (d'_{ij})$.

If $1 < i \leq n$, then $d_{ij} = |t_j - t_i| = |t'_j - t'_i| = d'_{ij}$ holds for $1 < j \leq n$.

If $1 < i \leq n$, then $d_{i1} = t_i - t_1 < t'_i - t'_1 = d'_{i1}$.

If $i = 1$, then $d_{1j} = t_j - t_1 \leq t'_j - t'_1 = d'_{1j}$ holds for $1 \leq j \leq n$.

Thus, the result follows from Lemma 2.4. ∎

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