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On the Spectral Properties of Line Distance Matrices

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Abstract

In [1], the authors showed that a line distance matrix of size $n > 1$, associated with biological sequences, has one positive and $n-1$ negative eigenvalues. The energy $E(G)$ of a graph G is defined as the sum of the absolute values of the eigenvalues of G in [2]. Similarly, we obtain bounds on the energy of line distance matrix. The spread of the spectrum of line distance matrix is considered.

1 Introduction

Let $t = (t_1, t_2, \cdots, t_n)$, $t_1 < t_2 < \cdots < t_n$, $t_i \in R$, be a given position vector. A line distance matrix, associated with t is defined as [1]

$$D = (d_{ij})_{n\times n}, \text{ where } d_{ij} = |t_i - t_j|.$$

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A DNA sequence consists of four nucleotides A, T, G, C. The distances between of A (or distances between T, G, or C) are represented in a vector t. Then a line distance matrix is associated with the vector t. Similarly, the line distance matrices associated with nucleotides T, G and C can be obtained. Then the given DNA sequence can be partly represented by the four line distance matrices. In [1], the authors reported:

Theorem A [1] *Let $D \in \mathbb{R}^{n\times n}$ be a line distance matrix, associated with a vector t and let $D^{(i)} := D(1 : i, 1 : i)$, $i = 1, 2, \cdots, n$, be its principal submatrices. Let*

$$\lambda_i^{(i)} \le \lambda_{i-1}^{(i)} \le \cdots \le \lambda_2^{(i)} \le \lambda_1^{(i)}$$

be the eigenvalues of the matrix $D^{(i)}$. Then $\lambda_1^{(i)} > 0$, $\lambda_2^{(i)} < 0$ for $i > 1$ and $\lambda_1^{(1)} = 0$.

Let G be a simple graph with n vertices. The adjacency matrix $A(G)$ of G is a square matrix of order n, where (i, j)-entry is equal to 1 if the vertices v_i and v_j are adjacent, and is equal to 0 otherwise. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of G are said to be the eigenvalues of the graph. The energy of G is defined as [2]

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

Some more recent results on energy and energy-like quantities have been obtained [3, 4, 5, 6].

Analogy to the graph energy, the line distance energy of $D^{(i)}$ is defined as

$$E(D^{(i)}) = \sum_{j=1}^{i} |\lambda_j^{(i)}|.$$

For an $n \times n$ complex matrix M, the spread, denoted by $s(M)$, is defined as the diameter of its spectrum, $s(M) := max_{i,j}|\lambda_i - \lambda_j|$, where λ_i, λ_j are the two arbitrary eigenvalues and the maximum is taken over all pairs of eigenvalues of M. Then the spread of the line distance matrix $D^{(i)}$ is $s(D^{(i)}) = \lambda_1^{(i)} - \lambda_i^{(i)}$.

In the paper [1], G. Jaklič et al. studied the eigenvalues of line distance matrices and reported that their spectrum consists of only one positive and $n-1$ negative eigenvalues. Recently, literature on the spread of arbitrary matrix and graphs has received much attention [7, 8, 9].

In this paper, we obtain some bounds and properties of $E(D^{(i)})$ and $s(D^{(i)})$. We find that some properties of $s(D^{(i)})$ are similar to the spread of graphs.

2 Bounds of $E(D^{(i)})$

By using the similar ideas of Krattenthaler [10], the authors obtained:

Lemma 2.1. [10] *Let* $D^{(i)}$, $i = 1, 2, \cdots, n$, *be the principal submatrices of* D *and* $detD^{(i)}$ *the determinant of* $D^{(i)}$. *Then* $detD^{(i)} = (-1)^{i+1}2^{i-2}(t_i - t_1)\prod_{j=1}^{i-1}(t_{j+1} - t_j)$.

Lemma 2.2. *Let* $\lambda_1^{(i)}$ *be the largest eigenvalues of* $D^{(i)}$. *Then*

$$\lambda_1^{(i)} \geq (i-1)^{\frac{i-1}{i}}\Big[2^{i-2}(t_i - t_1)\prod_{j=1}^{i-1}(t_{j+1} - t_j)\Big]^{\frac{1}{i}}.$$

Proof. Note that trace$D^{(i)} = \sum_{j=1}^{i}\lambda_j^{(i)} = 0$. Then $\lambda_1^{(i)} = -\lambda_2^{(i)} - \cdots - \lambda_i^{(i)}$. (1)

By Theorem A, $\lambda_1^{(i)} > 0$ and $0 < -\lambda_2^{(i)} \leq \cdots \leq -\lambda_i^{(i)}$.

Using the arithmetic-geometric mean inequality,

$$\begin{aligned} \lambda_1^{(i)} &= -\lambda_2^{(i)} - \cdots - \lambda_i^{(i)} \\ &\geq (i-1)\Big[(-\lambda_2^{(i)})\cdots(-\lambda_i^{(i)})\Big]^{\frac{1}{i-1}} \\ &= (i-1)\Big[(-1)^{(i-1)}\lambda_2^{(i)}\cdots\lambda_i^{(i)}\Big]^{\frac{1}{i-1}} \\ &= (i-1)\Big[(-1)^{(i-1)}\frac{detD^{(i)}}{\lambda_1^{(i)}}\Big]^{\frac{1}{i-1}} \\ &= (i-1)\Big[\frac{|detD^{(i)}|}{\lambda_1^{(i)}}\Big]^{\frac{1}{i-1}}. \end{aligned}$$

Then $(\lambda_1^{(i)})^{\frac{i}{i-1}} \geq (i-1)|detD^{(i)}|^{\frac{1}{i-1}}$.

By Lemma 2.1, the result follows. ∎

Theorem 2.3. *Let* $t = (t_1, t_2, \cdots, t_n)$, $t_1 < t_2 < \cdots < t_n$, $t_i \in R$, *be a given position vector. Then* $E(D^{(i)}) = 2\lambda_1^{(i)} \geq 2(i-1)^{\frac{i-1}{i}}\Big[2^{i-2}(t_i - t_1)\prod_{j=1}^{i-1}(t_{j+1} - t_j)\Big]^{\frac{1}{i}}$.

Proof. By Lemma 2.2 and equality (1),

$$\begin{aligned} E(D^{(i)}) &= \textstyle\sum_{j=1}^{i}|\lambda_j^{(i)}| = \lambda_1^{(i)} - \lambda_2^{(i)} - \cdots - \lambda_i^{(i)} = 2\lambda_1^{(i)} \\ &\geq 2(i-1)^{\frac{i-1}{i}}\Big[2^{i-2}(t_i - t_1)\prod_{j=1}^{i-1}(t_{j+1} - t_j)\Big]^{\frac{1}{i}}. \end{aligned}$$ ∎

Cauchy's interlacing theorem [11], as the technique is used in [1], implies

$$\lambda_{i-1}^{(i-1)} \leq \lambda_{i-1}^{(i)} \leq \cdots \leq \lambda_2^{(i-1)} \leq \lambda_2^{(i)} \leq \lambda_1^{(i-1)} \leq \lambda_1^{(i)}.$$

Corollary 2.4. *Let* $D^{(i)}$ *and* $D^{(j)}$ *be two principal submatrices of* D.

Then $E(D^{(i)}) \leq E(D^{(j)})$ *for* $i \leq j$. *Specially,* D *has the largest energy among the principal submatrices of* D.

Proof. By Cauchy's interlacing theorem, $\lambda_1^{(i)} \leq \lambda_1^{(i+1)} \leq \cdots \leq \lambda_1^{(j)}$, for $i \leq j$.

Note that $E(D^{(i)}) = 2\lambda_1^{(i)}$. Then $E(D^{(i)}) \leq E(D^{(i+1)}) \leq \cdots \leq E(D^{(j)})$. ∎

The (k,k)−entry of $[D^{(i)}]^2$ is equal to $\sum_{j=1}^{i} d_{kj}d_{jk} = \sum_{j=1}^{i}(d_{kj})^2 = \sum_{j=1}^{i}|t_k - t_j|^2$.

Then $trac[D^{(i)}]^2 = \sum_{k=1}^{i}\sum_{j=1}^{i}|t_k - t_j|^2 = 2\sum_{1\leq k<j\leq i}|t_k - t_j|^2 := M_i$.

Lemma 2.5. *Let* $\lambda_1^{(i)}$ *be the largest eigenvalues of* $D^{(i)}$. *Then* $\lambda_1^{(i)} \leq \sqrt{\frac{i-1}{i}M_i}$.

Proof. Note that $M_i = trac[D^{(i)}]^2 = \sum_{j=1}^{i}(\lambda_j^{(i)})^2$. (2)

Observe that x^2 is a strictly convex function. Then

$$\sum_{j=2}^{i}\frac{1}{i-1}(\lambda_j^{(i)})^2 \geq \Big[\sum_{j=2}^{i}\frac{1}{i-1}\lambda_j^{(i)}\Big]^2$$

i.e.,

$$\sum_{j=2}^{i}(\lambda_j^{(i)})^2 \geq \frac{1}{i-1}\Big[\sum_{j=2}^{i}\lambda_j^{(i)}\Big]^2.$$

By equality (2),
$$M_i - (\lambda_1^{(i)})^2 \geq \frac{1}{i-1}\Big[\sum_{j=2}^{i}\lambda_j^{(i)}\Big]^2 = \frac{1}{i-1}(-\lambda_1^{(i)})^2.$$

Thus $M_i \geq \frac{i}{i-1}(\lambda_1^{(i)})^2$, i.e., $\lambda_1^{(i)} \leq \sqrt{\frac{i-1}{i}M_i}$. ∎

By Theorem 2.3 and Lemma 2.5, we have

Theorem 2.6. *Let* $D^{(i)}$ *be a principal submatrix of* D. *Then* $E(D^{(i)}) \leq 2\sqrt{\frac{i-1}{i}M_i}$.

Theorem 2.7. *Let* $D^{(i)}$ *be a principal submatrix of* D. *Then* $E(D^{(i)}) \geq \sqrt{M_i + i(i-1)(detD^{(i)})^{\frac{2}{i}}}$.

Proof. By the definition of $E(D^{(i)})$, then

$$\begin{aligned}\left[E(D^{(i)})\right]^2 = \Big(\sum_{j=1}^{i}|\lambda_j^{(i)}|\Big)^2 &= \sum_{j=1}^{i}\left(\lambda_j^{(i)}\right)^2 + 2\sum_{1\leq k<l\leq i}|\lambda_k^{(i)}||\lambda_l^{(i)}| \\ &= M_i + 2\sum_{1\leq k<l\leq i}|\lambda_k^{(i)}||\lambda_l^{(i)}| \\ &= M_i + \sum_{k\neq l}|\lambda_k^{(i)}||\lambda_l^{(i)}|. \qquad (3)\end{aligned}$$

By the arithmetic-geometric mean inequality,

$$\sum_{k\neq l}|\lambda_k^{(i)}||\lambda_l^{(i)}| \geq i(i-1)\Big(\prod_{k\neq l}|\lambda_k^{(i)}||\lambda_l^{(i)}|\Big)^{\frac{1}{i(i-1)}}$$

$$= i(i-1)\Big(\prod_{j=1}^{i}|\lambda_j^{(i)}|^{2(i-1)}\Big)^{\frac{1}{i(i-1)}} = i(i-1)\prod_{j=1}^{i}|\lambda_j^{(i)}|^{\frac{2}{i}} = i(i-1)(detD^{(i)})^{\frac{2}{i}}.$$

By (3), then $\left[E(D^{(i)})\right]^2 \geq M_i + i(i-1)(detD^{(i)})^{\frac{2}{i}}$, i.e.,

$E(D^{(i)}) \geq \sqrt{M_i + i(i-1)(detD^{(i)})^{\frac{2}{i}}}$. ∎

3 The spread of $D^{(i)}$

In [9], D.A. Gregory et al. proved:

Theorem B. *If H is a induced subgraph of G, then $s(G) \geq s(H)$.*

Similarly, we have

Theorem 3.1. *Let $D^{(i)}$ and $D^{(j)}$ be two principal submatrices of $D = D^{(n)}$.*

Then $s(D^{(i)}) \leq s(D^{(j)})$ for $i \leq j$ and D has the largest spread among principal submatrices.

Proof. By Theorem A, note that $\lambda_1^{(i)} > 0$ and $\lambda_2^{(i)} < 0$ for any $i \geq 2$.

Cauchy's interlacing theorem implies

$\lambda_i^{(i)} \leq \lambda_{i-1}^{(i-1)} \leq \lambda_{i-1}^{(i)} \leq \cdots \leq \lambda_2^{(i-1)} \leq \lambda_2^{(i)} \leq \lambda_1^{(i-1)} \leq \lambda_1^{(i)}$.

Then $s(D^{(j)}) = \lambda_1^{(j)} - \lambda_i^{(j)} \geq \lambda_1^{(j-1)} - \lambda_i^{(j-1)} \geq \cdots \geq \lambda_1^{(i)} - \lambda_i^{(i)} = s(D^{(i)})$. ∎

Theorem 3.2. *Let $D^{(i)}$ be a principal submatrix of $D = D^{(n)}$. Then $s(D^{(i)}) \leq \sqrt{2M_i}$.*

Proof. Note that $M_i - (\lambda_1^{(i)})^2 - (\lambda_i^{(i)})^2 = \sum_{j=2}^{i-1}(\lambda_j^{(i)})^2$

$$\geq \frac{1}{i-2}(\sum_{j=2}^{i-1}\lambda_j^{(i)})^2$$

$$= \frac{1}{i-2}(\lambda_1^{(i)} + \lambda_i^{(i)})^2. \tag{4}$$

By (4),

$(i-1)(\lambda_i^i)^2 + 2\lambda_1^{(i)}\lambda_i^{(i)} + (i-1)(\lambda_1^{(i)})^2 - (i-2)M_i \leq 0$. The quadratic in $\lambda_i^{(i)}$ has one positive and one negative root, and it follows that $-\lambda_i^{(i)} \leq \frac{\lambda_1^{(i)}}{i-1} + \sqrt{\frac{i-2}{i-1}M_i - \frac{i^2-2i}{(i-1)^2}(\lambda_1^{(i)})^2}$.

Then $s(D^{(i)}) = \lambda_1^{(i)} - \lambda_i^{(i)} \leq \lambda_1^{(i)} + \frac{-\lambda_1^{(i)}}{i-1} + \sqrt{\frac{i-2}{i-1}M_i - \frac{i^2-2i}{(i-1)^2}(\lambda_1^{(i)})^2}$

$$= \frac{i}{i-1}\lambda_1^{(i)} + \sqrt{\frac{i-2}{i-1}M_i - \frac{i^2-2i}{(i-1)^2}(\lambda_1^{(i)})^2}.$$

Let $f(x) = \frac{i}{i-1}x + \sqrt{\frac{i-2}{i-1}M_i - \frac{i^2-2i}{(i-1)^2}x^2}$ $(\lambda_1^{(i)} = x > 0)$.
Considering the first derivative,
$f'(x) = \frac{i}{i-1} - \frac{i}{i-1}\sqrt{\frac{i-2}{i-1}}\frac{x}{\sqrt{M_i - \frac{i}{i-1}x^2}} = \frac{i}{i-1} - \frac{i}{i-1}\sqrt{\frac{i-2}{i-1}}\frac{1}{\sqrt{\frac{M_i}{x^2} - \frac{i}{i-1}}}$.
Let $f'(x) = 0$. Then $x = \sqrt{\frac{1}{2}M_i}$. By Lemma 2.5, $\lambda_1^{(i)} \leq \sqrt{\frac{i-1}{i}M_i}$.
In the interval $[\sqrt{\frac{1}{2}M_i}, \sqrt{\frac{i-1}{i}M_i})$, $f'(x) \leq 0$ and $f(x)$ is a decreasing function on x.
Then $s(D^{(i)}) \leq f(\lambda_1^{(i)}) \leq f\left(\sqrt{\frac{1}{2}M_i}\right) = \sqrt{2M_i}$. ∎

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