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BOUNDS ON THE DISTANCE LAPLACIAN ENERGY OF GRAPHS

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Abstract. Let G be a simple connected graph, v_i its vertex, and D_i the sum of distances between v_i and the other vertices of G. Let $\delta_1, \delta_2, \ldots, \delta_n$ be the eigenvalues of the distance matrix $\mathbf{D}$ of G, and $\delta_1^L, \delta_2^L, \ldots, \delta_n^L$ the eigenvalues of the distance Laplacian matrix $\mathbf{D}^L$ of G. An earlier much studied quantity $E_D(G) = \sum_{i=1}^n |\delta_i|$ is the distance energy. We now define the distance Laplacian energy as $LE_D(G) = \sum_{i=1}^n \left|\delta_i^L - \frac{1}{n}\sum_{i=1}^n D_i\right|$, and obtain bounds for it.

1. Introduction

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The distance matrix $\mathbf{D} = \mathbf{D}(G)$ of G is defined so that its (i,j)-entry d_{ij} is equal to the distance of (= length of a shortest path between) the vertices v_i and v_j [3]. The eigenvalues $\delta_1, \delta_2, \ldots, \delta_n$ of $\mathbf{D}(G)$ are said to be the distance eigenvalues of the graph G and form its distance spectrum. The distance eigenvalues obey the following simple relations:

$$\sum_{i=1}^n \delta_i = 0 \qquad \text{and} \qquad \sum_{i=1}^n \delta_i^2 = 2s \tag{1.1}$$

where

$$s = \sum_{1\le i<j\le n} (d_{ij})^2. \tag{1.2}$$

For earlier studies of the distance spectrum see [5–7, 10, 18, 20, 26, 29, 30].

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The distance degree of the vertex v_i, denoted by D_i, is given by $D_i = \sum_{j=1}^{n} d_{ij}$. In what follows we assume that the vertices of the graph G are labeled so that $D_1 \geq D_2 \geq \cdots \geq D_n$. G is said to be k-distance regular if $D_i = k$ for all i.

The distance Laplacian matrix of a connected graph G has been recently defined by Aouchiche and Hansen [1] as

$$\mathbf{D}^L = \mathbf{D}^L(G) = \mathrm{diag}(D_i) - \mathbf{D}(G)$$

where $\mathrm{diag}(D_i)$ denotes the diagonal matrix of the distance degrees. Since $\mathbf{D}^L$ is real symmetric, all its eigenvalues $\delta_i^L(G)$, $i = 1, 2, \ldots, n$, are real and can be labeled so that $\delta_1^L(G) \geq \delta_2^L(G) \geq \cdots \geq \delta_n^L(G)$. These form the distance Laplacian spectrum of G. If confusion is avoided, we shall write δ_i^L instead of $\delta_i^L(G)$.

Let $\phi_D^G(\lambda)$ and $\phi_L^G(\lambda)$ be, respectively, the characteristic polynomials of the distance matrix and the distance Laplacian matrix. In [1], $\phi_L^G(\lambda)$ has been calculated for some particular graphs, including the complete graph K_n, the complement of an edge $K_n - e$, the complete bipartite graph $K_{a,b}$, and the graph S_n^+, obtained by adding an edge to the star S_n. Results on $\delta_{n-1}^L(G)$, which is similar to the algebraic connectivity, have been obtained [1]. Moreover, the equivalence between the Laplacian spectrum and the distance Laplacian spectrum in the set of connected graphs with diameter 2 has also been demonstrated [1].

The following results from [1] will be needed.

Lemma 1.1. [1] *If $\{\delta_1, \delta_2, \ldots, \delta_n\}$ is the distance spectrum of a k-distance regular graph G, then $\{k - \delta_n, k - \delta_{n-1}, \ldots, k - \delta_1\}$ is the distance Laplacian spectrum of G.*

It is known that Laplacian eigenvalues of a graph interlace the Laplacian eigenvalues of its edge-deleted subgraph. Such an interlacing does not apply to the distance Laplacian spectrum [1]. Instead of it, one has the following.

Theorem 1.1. [1] *Let G be a connected graph of order n, with $m \geq n$ edges, and let $\tilde{G}$ be a connected graph obtained by deleting an edge from G. Let $\{\delta_1^L, \delta_2^L, \ldots, \delta_n^L\}$ and $\{\tilde{\delta}_1^L, \tilde{\delta}_2^L, \ldots, \tilde{\delta}_n^L\}$ be, respectively, the distance Laplacian spectra of G and $\tilde{G}$. Then $\tilde{\delta}_i^L \geq \delta_i^L$ holds for all $1 \leq i \leq n$.*

Corollary 1.1. [1] *Let G be a connected graph on n vertices. Then $\tilde{\delta}_i^L(G) \geq \delta_i^L(K_n)$ for all $1 \leq i \leq n-1$, and $\tilde{\delta}_n^L(G) = \delta_n^L(K_n) = 0$.*

The distance energy of a connected graph G was defined in [12] as

$$E_D(G) = \sum_{i=1}^{n} |\delta_i|.$$

For more results on $E_D(G)$, we refer readers to the references [2, 4, 7, 10–13, 21–24, 27, 28, 30].

In this paper, we define the distance Laplacian energy $LE_D(G)$, and show that it preserves the main features of distance energy.

2. Distance Laplacian energy

Our intention is to conceive a graph-energy-like quantity [17], defined in terms of distance Laplacian eigenvalues, that would preserve the main features of the distance energy. Bearing in mind relations (1.1), we first introduce the auxiliary "eigenvalues" ξ_i, defined as

$$\xi_i = \delta_i^L - \frac{1}{n}\sum_{j=1}^{n} D_j .$$

The trace of a matrix $\mathbf{X} = (x_{ij})_{n\times n}$ is defined as $tr(\mathbf{X}) = \sum_{i=1}^{n} x_{ii}$. It is also equal to the sum of eigenvalues of $\mathbf{X}$.

Lemma 2.1. *Let G be a connected graph of order n. Then $\sum_{i=1}^{n} \xi_i = 0$ and $\sum_{i=1}^{n} \xi_i^2 = 2S$, where*

$$S = s + \frac{1}{2}\sum_{i=1}^{n}\left(D_i - \frac{1}{n}\sum_{j=1}^{n} D_j\right)^2$$

and where s is given by Eq. (1.2).

Proof. Note that

$$\sum_{i=1}^{n} \delta_i^L = tr(\mathbf{D}^L) = \sum_{i=1}^{n} D_i$$

and

$$\sum_{i=1}^{n} (\delta_i^L)^2 = tr[(\mathbf{D}^L)^2] = \sum_{i=1}^{n} D_i^2 + \sum_{i,j=1}^{n} (d_{ij})^2 = \sum_{i=1}^{n} D_i^2 + 2s$$

from which we have

$$\sum_{i=1}^{n} \xi_i = \sum_{i=1}^{n}\left(\delta_i^L - \frac{1}{n}\sum_{j=1}^{n} D_j\right) = \sum_{i=1}^{n}\delta_i^L - \sum_{j=1}^{n} D_j = 0$$

and

$$\begin{aligned}\sum_{i=1}^{n} \xi_i^2 &= \sum_{i=1}^{n}\left(\delta_i^L - \frac{1}{n}\sum_{j=1}^{n} D_j\right)^2 \\ &= \sum_{i=1}^{n}(\delta_i^L)^2 - \frac{2}{n}\sum_{j=1}^{n} D_j \sum_{i=1}^{n}\delta_i^L + \frac{1}{n}\left(\sum_{j=1}^{n} D_j\right)^2 \\ &= \sum_{i=1}^{n} D_i^2 + 2s - \frac{2}{n}\left(\sum_{j=1}^{n} D_j\right)^2 + \frac{1}{n}\left(\sum_{j=1}^{n} D_j\right)^2 \\ &= 2s + \sum_{i=1}^{n}\left(D_i - \frac{1}{n}\sum_{j=1}^{n} D_j\right)^2 = 2S.\end{aligned}$$

□

Note that the equality $S = s$ holds if and only if G is distance regular.

Definition 2.1. Let G be a connected graph of order n. Then the distance Laplacian energy of G, denoted by $LE_D(G)$, is defined as $\sum_{i=1}^{n} |\xi_i|$, i.e.,

$$LE_D(G) = \sum_{i=1}^{n} \left| \delta_i^L - \frac{1}{n} \sum_{j=1}^{n} D_j \right|.$$

Example 2.1. $LE_D(K_n)$, $LE_D(K_n - e)$.

Since $\phi_L^{K_n}(\lambda) = \lambda(\lambda-n)^{n-1}$ [1], the distance Laplacian spectrum of K_n is $\{n^{[n-1]}, 0\}$, where $\omega^{[t]}$ means that ω is an eigenvalue with multiplicity t. Thus,

$$LE_D(K_n) = \sum_{i=1}^{n} \left| \delta_i^L(K_n) - \frac{1}{n} \sum_{j=1}^{n} D_j(K_n) \right| = \sum_{i=1}^{n} \left| \delta_i^L(K_n) - \frac{n(n-1)}{n} \right| = 2(n-1).$$

Since $\phi_L^{K_n - e}(\lambda) = \lambda(\lambda - n - 2)(\lambda - n)^{n-2}$ [1], the distance Laplacian spectrum of $K_n - e$ is $\{n+2, n^{[n-2]}, 0\}$. By direct calculation, $D_1 = D_2 = n$, $D_3 = D_4 = \cdots = D_n = n-1$, and therefore $\frac{1}{n} \sum_{j=1}^{n} D_j = \frac{n^2-n+2}{n} = n + \frac{2}{n} - 1$. Thus,

$$\begin{aligned} LE_D(K_n - e) &= \sum_{i=1}^{n} \left| \delta_i^L(K_n - e) - \frac{1}{n} \sum_{j=1}^{n} D_j(K_n - e) \right| \\ &= \sum_{i=1}^{n} \left| \delta_i^L(K_n - e) - \left(n + \frac{2}{n} - 1\right) \right| = 2\left(n + \frac{2}{n} - 1\right). \end{aligned}$$

Lemma 2.2. *If G is k-distance regular, then $LE_D(G) = E_D(G)$.*

Proof. Since G is k-distance regular, then $k = D_i = \frac{1}{n} \sum_{j=1}^{n} D_j$ for $i = 1, 2, \dots, n$. By Lemma 1.1,

$$\xi_i = \delta_i^L - \frac{1}{n} \sum_{j=1}^{n} D_j = (k - \delta_{n+1-i}) - k = -\delta_{n+1-i}$$

for $i = 1, 2, \dots, n$.

Thus, the result follows from the definitions of the distance energy and the distance Laplacian energy. □

3. Estimating the distance Laplacian energy

Theorem 3.1. *Let G be a connected graph of order n, $n \geq 2$. Then*

$$2\sqrt{S} \leq LE_D(G) \leq \sqrt{2nS}. \tag{3.1}$$

Moreover, the left–hand side equality holds if and only if G is a connected graph with at most two positive distance Laplacian eigenvalues $p > \frac{1}{n} \sum_{i=1}^{n} D_i$ and $q = \frac{1}{n} \sum_{i=1}^{n} D_i \geq n$. The right–hand side equality holds if and only if G is a connected graph whose distance Laplacian spectrum is $\left\{(\frac{2}{n} \sum_{i=1}^{n} D_i)^{[n-1]}, 0\right\}$.

Proof. Consider the non-negative term $T = \sum_{i=1}^{n}\sum_{j=1}^{n}(|\xi_i| - |\xi_j|)^2$. By direct calculation,

$$T = 2n\sum_{i=1}^{n}|\xi_i|^2 - 2\left(\sum_{i=1}^{n}|\xi_i|\right)\left(\sum_{j=1}^{n}|\xi_j|\right) = 2n\cdot 2S - 2LE_D(G)^2 = 4nS - 2LE_D(G)^2.$$

Since $T \geq 0$, $4nS - 2LE_D(G)^2 \geq 0$, which implies $LE_D(G) \leq \sqrt{2nS}$ for $S > 0$.

From $\left(\sum_{i=1}^{n}\xi_i\right)^2 = 0$ and the fact that $S > 0$, we have

$$2S = \sum_{i=1}^{n}\xi_i^2 = \left(\sum_{i=1}^{n}\xi_i\right)^2 - 2\sum_{1\leq i<j\leq n}\xi_i\,\xi_j$$

$$= -2\sum_{1\leq i<j\leq n}\xi_i\,\xi_j = 2\left|\sum_{1\leq i<j\leq n}\xi_i\xi_j\right| \leq 2\sum_{1\leq i<j\leq n}|\xi_i||\xi_j|.$$

Thus,

$$LE_D(G)^2 = \left(\sum_{i=1}^{n}|\xi_i|\right)^2$$

$$= \sum_{i=1}^{n}|\xi_i|^2 + 2\sum_{1\leq i<j\leq n}|\xi_i||\xi_j| \geq 2S + 2S = 4S$$

which yields $LE_D(G) \geq 2\sqrt{S}$.

Bearing in mind the above considerations, we note that equality in the left–hand side inequality (3.1) holds if and only if there is at most one positive-valued and at most one negative-valued ξ_i, $i = 1, 2, \ldots, n$. By Lemma 1.1, we have $\xi_n = \delta_n^L - \frac{1}{n}\sum_{j=1}^{n}D_j = -\frac{1}{n}\sum_{j=1}^{n}D_j < 0$ and $\delta_i^L \geq n > 0$ for $i = 1, 2, \ldots, n-1$. This implies that $\xi_1 = \xi_2 = \cdots = \xi_r > 0$ and $\xi_{r+1} = \cdots = \xi_{n-1} = 0$, where $r \in \{0, 1, 2, \cdots, n-1\}$. The case $r = 0$ means that $\xi_1 = \xi_2 = \ldots = \xi_{n-1} = 0$. Hence, in the set $\{\delta_1^L, \delta_2^L, \ldots, \delta_{n-1}^L\}$ there are at most two positive–valued elements $p > \frac{1}{n}\sum_{j=1}^{n}D_j$ and $q = \frac{1}{n}\sum_{j=1}^{n}D_j \geq n$.

In addition, we note that equality in the right–hand side inequality (3.1) holds if and only if $T = 0$, i.e., $|\xi_i| = |\xi_j|$ for $i, j = 1, 2, \ldots, n$. Thus $\delta_i^L = \frac{2}{n}\sum_{j=1}^{n}D_j$, $i = 1, 2, \ldots, n-1$, since

$$|\xi_n| = \left|\delta_n^L - \frac{1}{n}\sum_{i=1}^{n}D_i\right| = \frac{1}{n}\sum_{i=1}^{n}D_i$$

and $\delta_i^L \geq n > 0$ for $i = 1, 2, \ldots, n-1$. □

Note that K_n is a graph with exactly one positive distance Laplacian eigenvalue $n > \frac{1}{n}\sum_{i=1}^{n}D_i = n-1$. Therefore, $LE_D(K_n) = 2\sqrt{S}$. In addition, for $n \geq 3$,

$K_n - e$ is a graph with exactly two positive distance Laplacian eigenvalues $n+2$, n. Therefore, $LE_D(K_n - e) \neq 2\sqrt{S}$ since $n \neq \frac{1}{n}\sum_{i=1}^{n} D_i = n + \frac{2}{n} - 1$.

Corollary 3.1. *Let G be a connected graph of order n. Then $LE_D(G) \geq \sqrt{2n(n-1)}$.*

Proof. By Theorem 3.1 and $d_{ij} \geq 1$ for $i, j = 1, 2, \dots, n$,

$$LE_D(G) \geq 2\sqrt{S} = \sqrt{\sum_{1\leq i<j\leq n} (d_{ij})^2 + \frac{1}{2}\sum_{i=1}^{n}\left(D_i - \frac{1}{n}\sum_{j=1}^{n} D_j\right)^2}$$

$$\geq 2\sqrt{\sum_{1\leq i<j\leq n} (d_{ij})^2} \geq 2\sqrt{\binom{n}{2}} \geq \sqrt{2n(n-1)}.$$

□

The diameter of G, denoted by $\operatorname{diam}(G)$, is the maximum distance between any two vertices of G.

Corollary 3.2. *Let G be a connected (n,m)-graph with* $\operatorname{diam}(G) = 2$. *Then*

$$LE_D(G) \geq 2\sqrt{2n^2 - 2n - 3m}.$$

Proof. Since $\operatorname{diam}(G) = 2$, $d_{ij} = 1$ if $v_iv_j \in E(G)$ and $d_{ij} = 2$ if $v_iv_j \notin E(G)$. By Theorem 3.1, we have

$$LE_D(G) \geq 2\sqrt{S} = 2\sqrt{\sum_{1\leq i<j\leq n} (d_{ij})^2 + \frac{1}{2}\sum_{i=1}^{n}\left(D_i - \frac{1}{n}\sum_{i=1}^{n} D_i\right)^2}$$

$$\geq 2\sqrt{\sum_{1\leq i<j\leq n} (d_{ij})^2} = 2\sqrt{m \cdot 1^2 + \left[\frac{n(n-1)}{2} - m\right] \cdot 2^2}$$

$$= 2\sqrt{2n^2 - 2n - 3m}.$$

□

Lemma 3.1. [14] *Let $a_1, a_2, \dots, a_n$ be non-negative numbers. Then*

$$n\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{1/n}\right] \leq n\sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n}\sqrt{a_i}\right)^2$$

$$\leq n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{1/n}\right].$$

Theorem 3.2. *Let G be a connected graph with n vertices, $\mathbf{I}_n$ the unit matrix of order n, and*

$$\Delta = \left| \det \left(\mathbf{D}^L - \frac{1}{n} \sum_{i=1}^{n} D_i \, \mathbf{I}_n \right) \right| .$$

Then

$$\sqrt{2S + n(n-1)\Delta^{2/n}} \leq LE_D(G) \leq \sqrt{2(n-1)S + n\,\Delta^{2/n}}. \tag{3.2}$$

Proof. The bounds (3.2) are special cases of a result from [8]. For the sake of completeness, we sketch their proof.

Let $a_i = \xi^2$, $i = 1, 2, \ldots, n$, and

$$K = n \left[\frac{1}{n} \sum_{i=1}^{n} \xi_i^2 - \left(\prod_{i=1}^{n} \xi_i^2 \right)^{1/n} \right] \geq 0.$$

Then by Lemma 3.1,

$$K \leq n \sum_{i=1}^{n} \xi_i^2 - \left(\sum_{i=1}^{n} |\xi_i| \right)^2 \leq (n-1)K$$

that is, $K \leq 2nS - LE_D(G)^2 \leq (n-1)K$.

Since

$$K = n \left[\frac{2}{n} S - \left(\prod_{i=1}^{n} |\xi_i| \right)^{2/n} \right] = 2S - n\Delta^{2/n}$$

and

$$2S - n\Delta^{2/n} \leq 2nS - LE_D(G)^2 \leq (n-1)(2S - n\Delta^{2/n})$$

we arrive at the desired result. □

Remark 3.1. The upper bound of $LE_D(G)$ in Theorem 3.2 is always better than the one in Theorem 3.1. By $K \geq 0$, we have

$$2S = \sum_{i=1}^{n} \xi_i^2 = \sum_{i=1}^{n} |\xi_i|^2 \geq n \left(\prod_{i=1}^{n} |\xi_i|^2 \right)^{1/n} = n\,\Delta^{2/n}.$$

Thus,

$$\sqrt{2(n-1)S + n\Delta^{2/n}} \leq \sqrt{2nS}.$$

From the proof of Theorem 3.1, the equality

$$\sqrt{2(n-1)S + n\Delta^{2/n}} = \sqrt{2nS}$$

holds if and only if $|\xi_1| = |\xi_2| = \ldots = |\xi_n|$, i.e., if and only if G is a connected graph whose distance Laplacian spectrum is

$$\left\{ \left(\frac{2}{n} \sum_{i=1}^{n} D_i \right)^{[n-1]}, 0 \right\}.$$

Emulating a method invented by Koolen and Moulton [15, 16], and originally applied to the ordinary graph energy, we can formulate the following.

Theorem 3.3. *Let G be a connected graph of order n. Then*

$$LE_D(G) \leq \frac{1}{n} \sum_{i=1}^{n} D_i + \sqrt{(n-1) \left[2S - \left(\frac{1}{n} \sum_{i=1}^{n} D_i \right)^2 \right]}. \tag{3.3}$$

Proof. By Lemma 1.1, $\xi_n = 0 - \frac{1}{n} \sum_{i=1}^{n} D_i = -\frac{1}{n} \sum_{i=1}^{n} D_i$. Consider the non-negative term $T' = \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} (|\xi_i| - |\xi_j|)^2$. By direct calculation,

$$\begin{aligned} T' &= 2(n-1) \sum_{i=1}^{n-1} |\xi_i|^2 - 2 \left(\sum_{i=1}^{n-1} |\xi_i| \right) \left(\sum_{j=1}^{n-1} |\xi_j| \right) \\ &= 2(n-1) \left[2S - \left(\frac{1}{n} \sum_{i=1}^{n} D_i \right)^2 \right] - 2 \left(LE_D(G) - \frac{1}{n} \sum_{i=1}^{n} D_i \right)^2 \geq 0 \end{aligned}$$

which straightforwardly leads to inequality (3.3). □

Definition 3.1. [19] Let $(a) = (a_1, a_2, \ldots, a_r)$ and $(b_1, b_2, \ldots, b_s)$ be nonincreasing sequences of real numbers. Then (a) majorizes (b) if (a) and (b) satisfy the conditions:

$$\sum_{i=1}^{k} a_i \geq \sum_{i=1}^{k} b_i \quad \text{for} \quad k = 1, 2, \ldots, \min\{r, s\}, \text{ and} \tag{1}$$

$$\sum_{i=1}^{r} a_i = \sum_{i=1}^{s} b_i \,. \tag{2}$$

Remark 3.2. The upper bound for $LE_D(G)$ in Theorem 3.3 is always better than the one in Theorem 3.1. By applying the Cauchy–Schwartz inequality to the two $(n-1)$-dimensional vectors $(1, 1, \ldots, 1)$ and $(|\xi_2|, |\xi_3|, \ldots, |\xi_n|)$, we get

$$\left(\sum_{i=2}^{n} |\xi_i| \right)^2 \leq (n-1) \sum_{i=2}^{n} |\xi_i|^2$$

that is,

$$(LE_D(G) - |\xi_1|)^2 \leq (n-1)(2S - |\xi_1|^2)$$

and therefore

$$LE_D(G) \le |\xi_1| + \sqrt{(n-1)(2S - |\xi_1|^2)}. \tag{3.4}$$

It was proven in [25] that the spectrum of a positive semidefinite Hermitian matrix majorizes its main diagonal (when both are rearranged in nonincreasing order). By Lemma 1.1, $\mathbf{D}^L$ is a positive semidefinite matrix since $\delta_i^L(G) \ge 0$ for all $1 \le i \le n$. Noting that $\mathbf{D}^L$ is also symmetric, we have $\delta_1^L \ge D_1$ and $\xi_1 = \delta_1^L - \frac{1}{n}\sum_{i=1}^n D_i \ge D_1 - \frac{1}{n}\sum_{i=1}^n D_i \ge 0$. Thus Eq. (3.4) can be written as

$$LE_D(G) \le \xi_1 + \sqrt{(n-1)(2S - \xi_1^2)}.$$

Define the function $f(x) = x + \sqrt{(n-1)(2S - x^2)}$ for $x \ge 0$. By simple calculus, it can be shown that $f(x)$ is decreasing in the internal $\left[\sqrt{2S/n}, +\infty\right]$, and increasing in the internal $\left[0, \sqrt{2S/n}\right]$. Then

$$\begin{aligned} f\left(\sqrt{\frac{1}{n}\sum_{i=1}^n D_i}\right) &= \frac{1}{n}\sum_{i=1}^n D_i + \sqrt{(n-1)\left[2S - \left(\frac{1}{n}\sum_{i=1}^n D_i\right)^2\right]} \\ &\le \sqrt{2nS} = f\left(\sqrt{2S/n}\right) = f(x)_{\max}. \end{aligned}$$

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