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Ghodratollah Aalipour
alipour.ghodratollah@gmail.com

Aida Abiad
aidaabiad@gmail.com

Zhanar Berikkyzy
zhanarb@iastate.edu

Leslie Hogben
Iowa State University, hogben@aimath.org

Franklin H.J. Kenter
franklin.kenter@gmail.com

See next page for additional authors

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Authors

Ghodratollah Aalipour, Aida Abiad, Zhanar Berikkyzy, Leslie Hogben, Franklin H.J. Kenter, Jephian C.-H. Lin, and Michael Tait

PROOF OF A CONJECTURE OF GRAHAM AND LOVÁSZ CONCERNING UNIMODALITY OF COEFFICIENTS OF THE DISTANCE CHARACTERISTIC POLYNOMIAL OF A TREE*

GHODRATOLLAH AALIPOUR†, AIDA ABIAD‡, ZHANAR BERIKKYZY§, LESLIE HOGBEN¶,
FRANKLIN H.J. KENTER‖, JEPHIAN C.-H. LIN§, AND MICHAEL TAIT#

Abstract. The conjecture of Graham and Lovász that the (normalized) coefficients of the distance characteristic polynomial of a tree are unimodal is proved; it is also shown that the (normalized) coefficients are log-concave. Upper and lower bounds on the location of the peak are established.

Key words. Distance matrix, Characteristic polynomial, Unimodal, Log-concave.

AMS subject classifications. 05C50, 05C12, 05C31, 15A18.

1. Introduction. The *distance matrix* $\mathcal{D}(G)$ of a simple, finite, undirected, connected graph G is the matrix indexed by the vertices of G with (i,j)-entry equal to the distance between the vertices v_i and v_j, i.e., the length of a shortest path between v_i and v_j. The characteristic polynomial of $\mathcal{D}(G)$ is defined by $p_{\mathcal{D}(G)}(x) = \det(xI - \mathcal{D}(G))$ and is called the *distance characteristic polynomial* of G. Since $\mathcal{D}(G)$ is a real symmetric matrix, all of the roots of the distance characteristic polynomial are real. Distance matrices were introduced in the study of a data communication problem in [9]. This problem involves finding appropriate addresses so that a message can move efficiently through a series of loops from its origin to its destination, choosing the best route at each switching point. Recently, there has been renewed interest in the loop switching problem [6]. There has also been extensive work on distance spectra; see [1] for a recent survey.

A sequence $a_0, a_1, a_2, \ldots, a_n$ of real numbers is *unimodal* if there is a k such that $a_{i-1} \leq a_i$ for $i \leq k$ and $a_i \geq a_{i+1}$ for $i \geq k$, and the sequence is *log-concave* if $a_j^2 \geq a_{j-1}a_{j+1}$ for all $j = 1, \ldots, n-1$. Recent surveys about unimodality and related topics can be found in [2, 3], and a classical presentation is given in [5].

For a graph G on n vertices, the coefficient in $\det(\mathcal{D}(G) - xI) = (-1)^n p_{\mathcal{D}(G)}(x)$ of x^k is denoted by $\delta_k(G)$ by Graham and Lovász [8], so the coefficient of x^k in $p_{\mathcal{D}(G)}(x)$ is $(-1)^n \delta_k(G)$. The following statement appears on page 83 in [8] (a *tree* is a connected graph that does not have cycles, and n is its *order*, i.e., number of vertices):

> *It appears that in fact for each tree T, the quantities $(-1)^{n-1}\delta_k(T)/2^{n-k-2}$ are unimodal with the maximum value occurring for $k = \lfloor \frac{n}{2} \rfloor$. We see no way to prove this, however.*

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†Department of Mathematics and Computer Sciences, Kharazmi University, 50 Taleghani St., Tehran, Iran and Department of Mathematical and Statistical Sciences, University of Colorado Denver, CO, USA (alipour.ghodratollah@gmail.com).
‡Department of Econometrics and Operations Research, Tilburg University, Tilburg, The Netherlands (aidaabiad@gmail.com).
§Department of Mathematics, Iowa State University, Ames, IA 50011, USA (zhanar@ucr.edu).
¶Department of Mathematics, Iowa State University, Ames, IA 50011, USA, and American Institute of Mathematics, 600 E. Brokaw Road, San Jose, CA 95112, USA (hogben@aimath.org).
‖Mathematics Department, United States Naval Academy, Chauvenet Hall, 572C Holloway Road, Annapolis, MD 21402, USA (franklin.kenter@gmail.com).
#Department of Mathematics, University of California San Diego, La Jolla CA, 92037, USA (mtait@cmu.edu).

FACT 1.1. [8, equation (44)] *For a tree T on n vertices,*

$$(-1)^{n-1}\delta_k(T) > 0 \quad \text{for } 0 \le k \le n-2.$$

Throughout this discussion, the order of a graph is assumed to be at least three (any sequence a_0 is trivially unimodal and the peak location is 0). For a graph G of order n and $0 \le k \le n-2$, define $d_k(G) = |\delta_k(G)|/2^{n-k-2}$. We call the numbers $d_k(G)$ the *normalized coefficients*. If T is a tree, then $d_k(T) = (-1)^{n-1}\delta_k(T)/2^{n-k-2}$ by Fact 1.1. For a tree, the normalized coefficients represent counts of certain subforests of the tree [8]. The conjecture in [8] can be rephrased as:

> *For a tree T of order n, the sequence of normalized coefficients $d_0(T), \ldots, d_{n-2}(T)$ is unimodal and the peak occurs at $\left\lfloor \frac{n}{2} \right\rfloor$.*

The conjecture regarding the location of the peak was disproved by Collins [4] who showed that for both stars and paths the sequence $d_0(T), \ldots, d_{n-2}(T)$ is unimodal, but for paths the peak is at approximately $\left(1 - \frac{1}{\sqrt{5}}\right)n$ (and at $\left\lfloor \frac{n}{2} \right\rfloor$ for stars).[1] Conjecture 9 in [4], which Collins attributes to Peter Shor, is:

CONJECTURE 1.2. (Collins-Shor) *The [normalized] coefficients of the distance characteristic polynomial for any tree T with n vertices are unimodal with peak between $\left\lfloor \frac{n}{2} \right\rfloor$ and $\left\lceil \left(1 - \frac{1}{\sqrt{5}}\right)n \right\rceil$.*

In [4], Conjecture 9 is stated without the floor or ceiling; $\left\lfloor \frac{n}{2} \right\rfloor$ is clearly the intended lower bound, since [4, Theorem 1] establishes $\left\lfloor \frac{n}{2} \right\rfloor$ as the peak location for a star. An examination of the proof of [4, Theorem 3] shows that the ceiling is needed in the upper bound (although the path P_n may attain either the floor or the ceiling depending on n). This conjecture is included in [1] as Conjecture 2.6 (again without "normalized" and without the floor and ceiling), followed by the comment, *"No more results are known about that conjecture."*

The log-concavity of the sequences $d_k(T)$ of normalized coefficients and $|\delta_k(T)|$ of absolute values of coefficients are equivalent, and we show in Theorem 2.1 below that both sequences $|\delta_0(T)|, \ldots, |\delta_{n-2}(T)|$ and $d_0(T), \ldots, d_{n-2}(T)$ are log-concave and unimodal. In Section 3 we establish an upper bound of $\left\lceil \frac{2}{3}n \right\rceil$ for the peak location of the normalized coefficients. We also show that the coefficient $\frac{2}{3}$ can be improved when the tree is "star-like" with many paths of length 2. Further, we give a lower bound of $\frac{n}{d+1}$ where d is the diameter of the tree (i.e., the number of edges in a longest path in the tree). Finally, in Section 4 we give an example showing unimodality need not be true for graphs that are not trees.

To establish these results, we need some additional definitions and facts. The next observation is immediate from the definition.

OBSERVATION 1.3. *Let $a_0, a_1, a_2, \ldots, a_n$ be a sequence of real numbers, let c and s be nonzero real numbers, and define $b_k = sc^k a_k$. Then $a_0, a_1, a_2, \ldots, a_n$ is log-concave if and only if $b_0, b_1, b_2, \ldots, b_n$ is log-concave.*

Consider a real polynomial $p(x) = a_n x^n + \cdots + a_1 x + a_0$. The *coefficient sequence* of p is the sequence $a_0, a_1, a_2, \ldots, a_n$. The polynomial p is *real-rooted* if all roots of p are real (by convention, constant polynomials are considered real-rooted). The next result is known (see, for example, [2, 3, 5]). It is straightforward to adapt the proof of [2, Lemma 1.1] or [5, Theorem B, p. 270], which are stated with the additional assumption that the polynomial coefficients are nonnegative, to the more general case.

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[1] Despite use of the term *coefficient* throughout [4], the sequence discussed there is $d_k(T)$, not $\delta_k(T)$.

LEMMA 1.4.

(a) If $p(x) = a_n x^n + \cdots + a_1 x + a_0$ is a real-rooted polynomial, then:

 (i) $\frac{a_j^2}{\binom{n}{j}^2} \geq \frac{a_{j+1} a_{j-1}}{\binom{n}{j+1}\binom{n}{j-1}}$ for $j = 1, \ldots, n-1$.

 (ii) The coefficient sequence a_i of p is log-concave.

(b) If $a_0, a_1, a_2, \ldots, a_n$ is positive and log-concave, then $a_0, a_1, a_2, \ldots, a_n$ is unimodal.

2. Proof of Graham and Lovász' unimodality conjecture for the distance characteristic polynomial of a tree.

THEOREM 2.1. Let T be a tree of order n.

 (i) The coefficient sequence of the distance characteristic polynomial $p_{\mathcal{D}(T)}(x)$ is log-concave.

 (ii) The sequence $|\delta_0(T)|, \ldots, |\delta_{n-2}(T)|$ of absolute values of coefficients of the distance characteristic polynomial is log-concave and unimodal.

 (iii) The sequence $d_0(T), \ldots, d_{n-2}(T)$ of normalized coefficients of the distance characteristic polynomial is log-concave and unimodal.

Proof. Let $\mathcal{D}(T)$ be the distance matrix of T. Since $p_{\mathcal{D}(T)}(x)$ is real-rooted, the coefficient sequence $(-1)^n \delta_0(T), \ldots, (-1)^n \delta_{n-2}(T), 0, 1$ is log-concave by Lemma 1.4 (a) (i).

Therefore, the sequence $(-1)^n \delta_0(T), \ldots, (-1)^n \delta_{n-2}(T)$ is log-concave. By Fact 1.1, $(-1)^{n-1}\delta_k(T) > 0$ for $0 \leq k \leq n-2$, so we have $(-1)^n \delta_k(T) < 0$ for $0 \leq k \leq n-2$. Because all of the terms $(-1)^n \delta_0(T), \ldots, (-1)^n \delta_{n-2}(T)$ are negative, the sequence of their absolute values $\{|\delta_k(T)|\}_{k=0}^{n-2}$ is log-concave and positive. Then by Lemma 1.4 (b), the sequence $|\delta_0(T)|, \ldots, |\delta_{n-2}(T)|$ is unimodal.

Since $d_k(T) = \left(\frac{1}{2^{n-2}}\right) 2^k |\delta_k(T)|$, the log-concavity of the sequence $\{d_k(T)\}_{k=0}^{n-2}$ then follows from Observation 1.3. Since $\{d_k(T)\}_{k=0}^{n-2}$ is positive, it is unimodal by Lemma 1.4 (b). $\quad\square$

3. Bounds on the peak location.

For a tree T of order n, the question of the location of the peak of the unimodal sequence of normalized coefficients $\{d_k(T)\}_{k=0}^{n-2}$ remains open. Note that Conjecture 1.2 says that the peak location is between $\lfloor 0.5n \rfloor$ and roughly $\lceil 0.5528n \rceil$. Computations on *Sage* [10, 11] confirm this conjecture for all trees of order at most 20. In this section we show that the peak location is at most $\lceil 0.6667n \rceil$ for all trees of order n, and at least $\left\lfloor \frac{n-2}{1+d} \right\rfloor$ for a tree of diameter d and order n. Furthermore, the upper bound we establish is better for a "star-like" tree, that is, when the tree has a high fraction of the number of paths of length 2 in a star (which attains the maximum possible number of paths of length 2).

OBSERVATION 3.1. Let T be a tree on n vertices and define

$$\ell_T(x) = -\frac{1}{2^{n-2}} \det(2xI - \mathcal{D}(T)).$$

Then $\ell_T(x)$ is a real-rooted polynomial with coefficients -4 for x^n, 0 for x^{n-1}, and $d_k(T) > 0$ for x^k when $0 \leq k \leq n-2$.

LEMMA 3.2. Let $a_0, a_1, a_2, \ldots, a_{n-2}$ be a unimodal sequence with $a_i > 0$ for $i = 0, \ldots, n-2$ such that $\sum_{k=0}^n a_k x^k$ is a real-rooted polynomial.

 1. If for some index $j \neq n, n-1$

$$\frac{n-j}{n(j+1)} \cdot \frac{a_1}{a_0} < 1,$$

then the peak location is at most j.

2. *If for some index $j \neq n, n-1, 0$*

$$\frac{(n-2)(n-j+1)}{3j} \cdot \frac{a_{n-2}}{a_{n-3}} > 1,$$

then the peak location is at least j.

Proof. By Lemma 1.4 (a) (i),

$$a_j^2 \geq \frac{\binom{n}{j}^2}{\binom{n}{j+1}\binom{n}{j-1}} a_{j+1} a_{j-1} = \frac{(j+1)(n-j+1)}{j(n-j)} a_{j+1} a_{j-1}.$$

Then

$$\frac{a_{j+1}}{a_j} \leq \frac{j(n-j)}{(j+1)(n-j+1)} \cdot \frac{a_j}{a_{j-1}}$$

$$\leq \left(\frac{j}{j+1} \cdot \frac{j-1}{j} \cdots \frac{1}{2} \right) \left(\frac{n-j}{n-j+1} \cdot \frac{n-j+1}{n-j+2} \cdots \frac{n-1}{n} \right) \frac{a_1}{a_0}$$

$$= \frac{n-j}{n(j+1)} \cdot \frac{a_1}{a_0}.$$

If this value is smaller than 1, then $a_{j+1} < a_j$ and the peak location is at most j.

Similarly,

$$\frac{a_j}{a_{j-1}} \geq \frac{(j+1)(n-j+1)}{j(n-j)} \cdot \frac{a_{j+1}}{a_j}$$

$$\geq \left(\frac{j+1}{j} \cdot \frac{j+2}{j+1} \cdots \frac{n-2}{n-3} \right) \left(\frac{n-j+1}{n-j} \cdot \frac{n-j}{n-j-1} \cdots \frac{4}{3} \right) \frac{a_{n-2}}{a_{n-3}}$$

$$= \frac{(n-2)(n-j+1)}{3j} \cdot \frac{a_{n-2}}{a_{n-3}}.$$

If this value is greater than 1, then $a_j > a_{j-1}$ and the peak location is at least j. $\square$

THEOREM 3.3. *Suppose T is a tree on $n \geq 3$ vertices with at least $\rho\binom{n-1}{2}$ paths of length 2 for some nonnegative real number ρ. Then the peak location of the normalized coefficients $d_0(T), d_1(T), \ldots, d_{n-2}(T)$ is at most $\left\lceil \frac{2-\rho}{3-\rho} n \right\rceil$. Since $\rho = 0$ applies to every tree, the peak location is at most $\left\lceil \frac{2}{3}n \right\rceil$ for every tree on n vertices.*

Proof. By Observation 3.1, we may apply Lemma 3.2 to $\ell_T(x)$. When $0 \leq j \leq n-2$ and

$$\frac{n-j}{n(j+1)} \cdot \frac{d_1(T)}{d_0(T)} < 1,$$

the peak location is at most j. Since $d_0(T)$ and $d_1(T)$ are both positive numbers, the inequality is equivalent to

$$j > \frac{rn-n}{n+r} = n - \frac{n^2+n}{n+r}, \quad \text{where } r = \frac{d_1(T)}{d_0(T)}.$$

The formula $d_0(T) = n-1$ is given in [9, Theorem 3]. Defining $N_{P_3}(T)$ to be the number of subtrees of T that are isomorphic to the path P_3 on three vertices (of length 2), the formula $d_1(T) = 2n(n-1) - $

$2N_{P_3}(T) - 4$ follows from [7, Theorem 4.1][2] by using the definition $d_k(T) = (-1)^{n-1}\delta_k(T)/2^{n-k-2}$. Since $\frac{1}{2}\rho(n-1)(n-2) = N_{P_3}(T) \geq n - 2$,

$$r = \frac{2n(n-1) - 2N_{P_3}(T) - 4}{n-1} = \frac{2n(n-1) - \rho(n-1)(n-2) - 4}{n-1} < (2-\rho)n + 2\rho.$$

Now

$$n - \frac{n^2 + n}{n + r} < n - \frac{n^2 + n}{(3-\rho)n + 2\rho} = n - \frac{n+1}{3 - \rho + (2\rho/n)} \leq n - \frac{n}{3-\rho} = \frac{2-\rho}{3-\rho}n.$$

The last inequality follows from $\frac{n}{3-\rho} \leq \frac{1}{(2\rho/n)}$, which is justified by $\rho \leq 1$.

Therefore, $j = \left\lceil \frac{2-\rho}{3-\rho}n \right\rceil$ is an upper bound of the peak location.   □

REMARK 3.4. If the number $N_{P_3}(T)$ of paths of length two is known for every tree T in a particular family, then ρ can be set equal to $\frac{N_{P_3}(T)}{\binom{n-1}{2}}$. For example, for the star S_n on n vertices, $N_{P_3}(S_n) = \binom{n-1}{2}$, so $\rho = 1$ and $\left\lceil \frac{2-\rho}{3-\rho}n \right\rceil = \left\lceil \frac{n}{2} \right\rceil$. Thus, for a star, our upper bound is equal to (if n is even) or one more than (if n is odd) the known value $\left\lfloor \frac{n}{2} \right\rfloor$ for the peak of the normalized coefficients for S_n [4, Theorem 1].

We will utilize a technique similar to the upper bound in order to derive a lower bound. However, we need the following lemma to provide an estimate for the necessary ratio.

LEMMA 3.5. *For any tree T on n vertices with diameter d*

$$\frac{d_{n-3}(T)}{d_{n-2}(T)} < \frac{1}{3}nd.$$

Proof. Let $\mathcal{D} := \mathcal{D}(T)$ denote the distance matrix of T, and let $\mathcal{D}_{ij}$ denote its ij-entry. From [7, equations (4c) and (4d)],

$$\delta_{n-2}(T) = (-1)^{n-1}\sum_{i<j}\mathcal{D}_{ij}^2$$

and

$$\delta_{n-3}(T) = (-1)^{n-1}\sum_{i<j<k}2\mathcal{D}_{ij}\mathcal{D}_{jk}\mathcal{D}_{ki}.$$

We will now express the corresponding normalized coefficients in terms of the traces of powers of $\mathcal{D}$. First, let us consider $d_{n-2}(T)$. Since the diagonal entries of $\mathcal{D}$ are all zero,

$$d_{n-2}(T) = \sum_{i<j}\mathcal{D}_{ij}^2 = \frac{1}{2}\sum_i\sum_j\mathcal{D}_{ij}\mathcal{D}_{ji} = \frac{1}{2}\sum_i(\mathcal{D}^2)_{ii} = \frac{1}{2}\operatorname{tr}(\mathcal{D}^2),$$

---

[2] Our notation is slightly different but examination of [7, Table 2] clarifies the notation.

where the second equality follows from $\mathcal{D}$ being symmetric. Similarly, for $d_3(T)$,

$$
\begin{aligned}
d_{n-3}(T) &= \sum_{i<j<k} \mathcal{D}_{ij}\mathcal{D}_{jk}\mathcal{D}_{ki} \\
&= \frac{1}{6} \sum_{\substack{i,j,k \\ \text{different}}} \mathcal{D}_{ij}\mathcal{D}_{jk}\mathcal{D}_{ki} \\
&= \frac{1}{6} \sum_{i,j,k} \mathcal{D}_{ij}\mathcal{D}_{jk}\mathcal{D}_{ki} \\
&= \frac{1}{6} \sum_i \sum_{j,k} \mathcal{D}_{ij}\mathcal{D}_{jk}\mathcal{D}_{ki} = \frac{1}{6} \sum_i (\mathcal{D}^3)_{ii} = \frac{1}{6} \operatorname{tr}(\mathcal{D}^3),
\end{aligned}
$$

where the third line follows because if any two of i, j, k are equal, then the corresponding entry in $\mathcal{D}$ is 0.

Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n =: \lambda_{max}$ denote the eigenvalues of $\mathcal{D}(T)$. Since $\operatorname{tr}(\mathcal{D}^2) = \sum_i \lambda_i^2$ and similarly $\operatorname{tr}(\mathcal{D}^3) = \sum_i \lambda_i^3$, we have

$$
\frac{d_{n-3}(T)}{d_{n-2}(T)} = \frac{\frac{1}{6}\operatorname{tr}(\mathcal{D}(T)^3)}{\frac{1}{2}\operatorname{tr}(\mathcal{D}(T)^2)} = \frac{1}{3}\frac{\sum_i \lambda_i^3}{\sum_i \lambda_i^2} \leq \frac{1}{3}\frac{\lambda_{max}\sum_i \lambda_i^2}{\sum_i \lambda_i^2} = \frac{1}{3}\lambda_{max} < \frac{1}{3}nd,
$$

where the last inequality comes from that the the row sums of $\mathcal{D}$ are bounded above by nd.   □

THEOREM 3.6. *Let T be a tree on $n \geq 3$ vertices with diameter d. Then, the peak location of the normalized coefficients $d_0(T), d_1(T), \ldots, d_{n-2}(T)$ is at least $\left\lfloor \frac{n-2}{1+d} \right\rfloor$.*

Proof. By Observation 3.1, we may apply Lemma 3.2 to $\ell_T(x)$. When $1 \leq j \leq n-2$ and

$$
\frac{(n-2)(n-j+1)}{3j} \cdot \frac{d_{n-2}(T)}{d_{n-3}(T)} > 1,
$$

the peak location is at least j. Since $d_{n-2}(T)$ and $d_{n-3}(T)$ are both positive numbers, the inequality is equivalent to

$$
j < \frac{(n-2)(n+1)}{(n-2) + (3/r)}, \quad \text{where } r = \frac{d_{n-2}(T)}{d_{n-3}(T)}.
$$

By applying Lemma 3.5, $\frac{3}{r} < nd$. Thus,

$$
\begin{aligned}
\frac{(n-2)(n+1)}{(n-2)+(3/r)} &> \frac{(n-2)(n+1)}{(1+d)n-2} \\
&= \frac{n-2}{1+d} \cdot \frac{n+1}{n-2/(1+d)} \\
&> \frac{n-2}{1+d}.
\end{aligned}
$$

So, $j = \left\lfloor \frac{n-2}{1+d} \right\rfloor$ is a lower bound of the peak location.   □

4. Graphs that are not trees. Since the distance matrix of any graph G is a real symmetric matrix, the coefficient sequence of the distance characteristic polynomial of G is log-concave. However, it need not be the case that all coefficients of the distance characteristic polynomial have the same sign. Thus, statements analogous to those in Theorem 2.1 can be false for graphs that are not trees.

EXAMPLE 4.1. The normalized coefficients and absolute values of the coefficients of the distance characteristic polynomial are not unimodal (and hence not log-concave) for the Heawood graph H shown in Figure 1. The coefficients of the distance characteristic polynomial are log-concave but not unimodal.
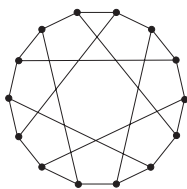

FIGURE 1. *The Heawood graph H.*

The distance characteristic polynomial of H is

$$p_{\mathcal{D}(H)}(x) = x^{14} - 441x^{12} - 6328x^{11} - 36456x^{10} - 75936x^9 + 104720x^8$$
$$+ 573696x^7 - 118272x^6 - 1885184x^5 + 973056x^4$$
$$+ 2795520x^3 - 3885056x^2 + 1892352x - 331776.$$

The values of $d_k(H)$, for $k = 0, \ldots, 12$, are

$$81, \ 924, \ 3794, \ 5460, \ 3801, \ 14728, \ 1848, \ 17928, \ 6545, \ 9492, \ 9114, \ 3164, \ 441.$$

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