Proof of a conjecture of Graham and Lovász concerning unimodality of coefficients of the distance characteristic polynomial of a tree

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Abstract

We establish a conjecture of Graham and Lovász that the (normalized) coefficients of the distance characteristic polynomial of a tree are unimodal; we also prove they are log-concave.

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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 [7]. 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 [5]. 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 $a_{i-1} \le a_i$ for $i \le k$ and $a_i \ge a_{i+1}$ for $i \ge k$, and the sequence is *log-concave* if $a_j^2 \ge a_{j-1}a_{j+1}$ for all $j = 1, \ldots, n-1$. Recent surveys about unimodality and related topics can be found in [2, 3].

For a graph G on n vertices, the coefficient of x^k in $\det(\mathcal{D}(G) - xI) = (-1)^n p_{\mathcal{D}(G)}(x)$ is denoted by $\delta_k(G)$ by Graham and Lovász [6], 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 [6] (n is the order of the tree):

> *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.*

Fact 1.1. [6, Equation (44)] *For a tree T on n vertices,*

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

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 $d_k(G) = \left(\frac{1}{2^{n-2}}\right) 2^k |\delta_k(G)|$. 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; in this case, the normalized coefficients represent counts of certain subforests of the tree [6]. The conjecture in [6] 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 $\lfloor \frac{n}{2} \rfloor$.*

The conjecture regarding the location of the peak was disproved by Collins [4] who showed that for both stars and paths the sequence $d_0(T), \dots, d_{n-2}(T)$ 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:

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

This conjecture is included in [1] as Conjecture 2.6, 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 $|\delta_0(T)|, \dots, |\delta_{n-2}(T)|$ and $d_0(T), \dots, d_{n-2}(T)$ are log-concave and unimodal. We also briefly discuss the peak location for the normalized coefficients in Section 3.1 and give an example showing unimodality need not be true for graphs that are not trees in Section 3.2.

To establish these results, we need some additional definitions and facts. Consider a real polynomial $p(x) = a_n x^n + \dots + a_1 x + a_0$. The *coefficient sequence* of p is the sequence $a_0, a_1, a_2, \dots, a_n$. The polynomial p is *real-rooted* if all roots of p are real (by convention, constant polynomials are considered real-rooted). The next observation is immediate from the definition.

Observation 1.2. *Let $a_0, a_1, a_2, \dots, a_n$ be a sequence of real numbers, let c and s be nonzero real numbers, and define $b_k = sc^k a_k$. Then $a_0, a_1, a_2, \dots, a_n$ is log-concave if and only if $b_0, b_1, b_2, \dots, b_n$ is log-concave.*

The next result is known (see, for example, [2, 3]). For completeness, we include the brief proof adapted from [2, Lemma 1.1] (where it is stated with the additional assumption that the polynomial coefficients are nonnegative).

Lemma 1.3.

(i) *If p is a real-rooted polynomial, then the coefficient sequence of p is log-concave.*

(ii) *If $a_0, a_1, a_2, \dots, a_n$ is positive and log-concave, then $a_0, a_1, a_2, \dots, a_n$ is unimodal.*

Proof. The second statement is immediate from the definitions. For a nonnegative integer m, let $m_{(\ell)}$ denote the coefficient of the ℓ-th derivative of x^m. If $q(x)$ is a polynomial of degree d with real roots, then its derivative is a real-rooted polynomial, and the polynomial $x^d q\left(\frac{1}{x}\right)$ also has real roots. Suppose $p(x) = a_n x^n + \dots + a_1 x + a_0$ is a real-rooted polynomial of degree $n \geq 2$. Fix j with $1 \leq j \leq n-1$. Define $f(x)$ to be the $(j-1)$th derivative of $p(x)$,

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

$g(x) = x^{n-j+1} f\left(\frac{1}{x}\right)$, and $h(x)$ to be the $(n-j-1)$th derivative of $g(x)$. Then $g(x) = \sum_{k=0}^{n} k_{(j-1)} a_k x^{n-k}$ and

$$\begin{aligned} h(x) &= \sum_{k=0}^{n} \left(k_{(j-1)}\right) \left((n-k)_{(n-j-1)}\right) a_k x^{j+1-k} \\ &= \frac{(j-1)!(n-j+1)!}{2} a_{j-1} x^2 + j!(n-j)! a_j x + \frac{(j+1)!(n-j-1)!}{2} a_{j+1} \\ &= \frac{n!}{2} \left(\frac{a_{j-1}}{\binom{n}{j-1}} x^2 + \frac{2a_j}{\binom{n}{j}} x + \frac{a_{j+1}}{\binom{n}{j+1}} \right). \end{aligned}$$

Since $h(x)$ has real roots, $\frac{a_j^2}{\binom{n}{j}^2} \geq \frac{a_{j+1}a_{j-1}}{\binom{n}{j+1}\binom{n}{j-1}}$, which implies $a_j^2 \geq a_{j+1}a_{j-1}$ because $\frac{\binom{n}{j}^2}{\binom{n}{j+1}\binom{n}{j-1}} > 1$ for all $1 \leq j \leq n-1$. □

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 1.3(i).

Therefore, $(-1)^n\delta_0(T), \ldots, (-1)^n\delta_{n-2}(T)$ 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 $0 \leq k \leq n-2$. Since 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 1.3(ii), 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 1.2. Since $\{d_k(T)\}_{k=0}^{n-2}$ is positive, it is unimodal by Lemma 1.3(ii). □

3. Further remarks

3.1. Peak location

The question of the location of the peak of the unimodal sequence of normalized coefficients $\{d_k(T)\}_{k=0}^{n-2}$ for a tree T remains open. Theorem 3 in [4] states:

The coefficients of [the distance characteristic polynomial] of a path on n vertices are unimodal with peak at $n(1 - \frac{1}{\sqrt{5}})$.

In fact, what is being discussed is the peak location for the normalized coefficients, and $\lfloor \frac{n}{2} \rfloor$ is clearly the intended lower bound. What is the intended interpretation of the (irrational) number $n\big(1 - \frac{1}{\sqrt{5}}\big)$? A careful examination of the proof of [4, Theorem 3] shows that the Collins/Shor Conjecture could be more precisely stated as:

For every tree T, the location of the peak of the unimodal sequence of normalized coefficients $\{d_k(T)\}_{k=0}^{n-2}$ is between $\lfloor \frac{n}{2} \rfloor$ and $\lceil n - \frac{n}{\sqrt{5}} \rceil$.

Computations on *Sage* [8, 9] confirm this conjecture for all trees of order at most 20.

3.2. 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 3.1. 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.

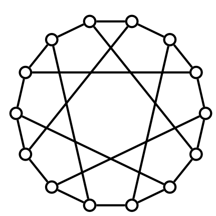

Figure 1: The Heawood graph H

The distance characteristic polynomial of H is

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

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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