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Terminal polynomials and star-like graphs

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Abstract

A terminal polynomial is the characteristic polynomial of the distance matrix between all pairs of leaves (valence one vertices) of a given graph. Two graphs are isoterminal if they share the same terminal polynomial. In this paper we prove the Clarke-type theorem about terminal polynomial of a given graph and prove that there are countably many isoterminal pairs of graphs. We investigate isoterminal pairs of star-like graphs in more details and calculate the isoterminal pair of star-like graphs with three rays that has the smallest number of vertices (in both graphs together) compared to all isoterminal pairs of star-like graphs with three rays.

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1 Introduction

Graphical representation of proteins, which are made of amino acids arranged in a linear chain, has been initiated only recently [10]. The sequence of amino acids in a protein is determined by the genetic code, which specifies the order in which the 20 natural amino acids occur. Among the latest development in this area is use of star-like graphs for construction of graphical representation of proteins [15]. Star graphs are connected graphs with at most one vertex of degree $d \geq 3$ and all other vertices of $d = 1$, while star-like graphs are connected graphs with with at most one vertex of degree $d \geq 3$ (while other vertices are of $d = 1$ and $d = 2$). In contrast to graphical representation of proteins graphical representation of DNA (deoxyribonucleic acid), which consists of four nucleic acids and determines the genetic information used in the development of all living organisms, has been around for 25 years [7]. Different history for graphical representation of proteins and DNA is due to combinatorial complexity accompanying ordering of 20 objects relative to that of four when considering use of labeled geometrical objects as template for their representation. However, graphs have here an important advantage in offering graphical representation of the same graph (protein) that may appear different, depending or order in which vertices are labeled, but which will lead to the same set of invariants regardless labeling of its vertices. Thus the quagmire of 20 factorials has been bypassed.

When star-like graphs are used for visual representation of proteins one is interested in graphs with at most 20 rays. Such graphs can be used unlabeled and labeled, with labels indicating the site in which amino acids appear in the sequence [10]. When graph invariants are considered as potential graph descriptors there is always loss of information, which is the reason that typically one considers set of invariants for their characterization. Among various invariants for characterization of molecular graphs [12] the leading eigenvalue and eigenvalues have been occasionally considered [14]. In such cases additional loss of information may occur due to possibility of isospectrality, the situation that different graphs may have the same characteristic polynomials and the same set of eigenvalues. Collatz and Sinogowitz were the first to report on a collection of isospectral trees [3]. Since then numerous results on isospectral (or cospectral) graphs have been reported, particularly in mathematical and chemical literature [16].

In view that star-like graphs have been proposed for graphical representation of proteins it is of interest to study their mathematical properties more closely, including spectral properties [4, 5, 8, 9]. In this contribution we will in particular focus on terminal polynomials of star-like graphs. Informally terminal polynomials are defined for trees and are the characteristic polynomials of the reduced distance matrix that involves only distances between terminal vertices. In a preliminary report Randić and Kleiner [11, 13] reported on a pair of simple star-like graphs, having only three rays, which have the same set of eigenvalues for the reduced distance matrix involving terminal vertices. We will refer to such graphs as isoterminal graphs, in analogy with the label isospectral graph, for graphs having the same characteristic polynomial. In this work we revisited the subject and made a more detailed study of isospectrality of terminal graphs and some other their properties.

Other, more mathematically oriented work that is connected to this subject is [1], where authors studied distance matrix realizability with trees (which matrices are terminal matrices of trees).

2 Definitions

All graphs in this paper are considered to be finite, undirected, connected and simple. We shall study special submatrices of distance matrices, called terminal distance matrices. Define $D(G)$ to be the graph-theoretical distance matrix of G and let $\mathcal{D}(G)$ be the graph-theoretical distance matrix of distances between all pairs of *terminal vertices* (or valence one vertices) of a graph G. We refer to $\mathcal{D}(G)$ as *terminal distance matrix* of G. It has been proved in [17] that any tree is completely defined by its terminal distance matrix.

Let G be a graph on $n = |V(G)|$ vertices and let I_n be the $n \times n$ identity matrix. The polynomial

$$\mathcal{P}_G(x) = \det(\mathcal{A}(G) - xI_n)$$

of the adjacency matrix $\mathcal{A}(G)$ of graph G, is called the *characteristic polynomial* of G. Similarly, the polynomial $\det(\mathcal{D}(G) - xI_N)$ of the terminal distance matrix $\mathcal{D}(G)$ of a graph G with N terminal vertices is called *terminal polynomial* of G. The information contained in the terminal polynomial may have practical use; for instance, the degree of the terminal polynomial tells us the number of vertices of valence one in a graph. In Section 3 we consider terminal polynomials and prove Clarke-type theorem (see [2]) for terminal polynomials.

Let $N > 0$ be a natural number and let $a = \{a_1, a_2, \ldots, a_N\}$ be a tuple of positive integers, such that $\forall i,\ a_i \geq 1$. A *star-like graph* $\mathcal{S}(a)$ with N rays is a graph with vertex set $V(\mathcal{S}(a)) = \{u\} \cup \{v_{i,j}, 1 \leq i \leq N, 1 \leq j \leq a_i\}$ and edge set $E(\mathcal{S}(a)) = \{u \sim v_{i,1}, 1 \leq i \leq N\} \cup \{v_{i,j} \sim v_{i,j-1}, 1 \leq i \leq N, 2 \leq j \leq a_i\}$. Thus $|V(\mathcal{S}(a))| = 1 + \sum_{j=1}^{N} a_j$ and $|E(\mathcal{S}(a))| = \sum_{j=1}^{N} a_j$. Figure 1 depicts the star-like graph $\mathcal{S}(\{1, 2, 3\})$ with three rays. The induced subgraph of $\mathcal{S}(a)$ on vertex set $\{v_{i,j} \sim v_{i,j-1}, 2 \leq j \leq a_i\}$ will be called i-th *ray*.

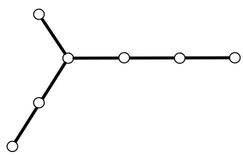


Figure 1: The star-like graph $\mathcal{S}(\{1, 2, 3\})$.

Section 4 considers graphs with the same terminal polynomial, the so-called isoterminal graphs. We prove that there is countably many isoterminal graphs and define ireducible and reducible graphs. In Section 5 we observe star-like graphs on three rays. We obtain the smallest isoterminal pair of star-like graphs with three rays; the smallest in a way, that the sum of the vertices of both graphs is the smallest among all isoterminal pairs of star-like graphs on three rays. We calculated all ireducible isoterminal pairs of star-like graphs with three rays, for which the smallest graph in the pair has all rays of length up to 200 vertices.

3 Terminal polynomial

Let G be a graph and let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of the graph G. The (Ulam) subgraph of G induced by the vertex set $V(G) \setminus \{v_i\}$ will be denoted by $G_{(i)}$.

Let $\mathcal{A}(G, \ell)$ be the *labeled adjacency matrix* of a graph G using the edge labeling ℓ, that is, the $|V(G)| \times |V(G)|$ symmetric matrix whose ij-th entry is $\ell(e)$, if v_i and v_j are joined by an edge $e = v_i \sim v_j$, and 0 otherwise; for analogous definition, see [2]. From labeling all edges with label $\ell(x) = 1$ the well known adjacency matrix $\mathcal{A}(G) := \mathcal{A}(G, 1)$ is obtained. As in [2], define the polynomial

$$\mathcal{R}_{G,\ell}(x) = \det(\mathcal{A}(G, \ell) + xI_n),$$

of the labeled adjacency matrix $\mathcal{A}(G, \ell)$ of the graph G using edge labeling ℓ, where again, I_n is the $n \times n$ identity matrix.

Lemma 3.1. *Let G be a graph with edge labeling ℓ, let $n = |V(G)|$ and let $G_{(i)}$, $1 \leq i \leq n$, be its Ulam subgraphs. Then*

$$\frac{\partial\ \mathcal{R}_{G,\ell}(x)}{\partial x} = \sum_{i=1}^{n} \mathcal{R}_{G_{(i)},\ell}(x).$$

Proof. We can prove our theorem following the idea that proves Theorem 2 and Corollary 3 in [2] and considering labeling of the edges throughout the proof. □

Corollary 3.2. *Let $\mathcal{P}_{G,\ell}(x) = \det(\mathcal{A}(G, \ell) - xI_n)$ be the characteristic polynomial of* *the labeled adjacency matrix $\mathcal{A}(G,\ell)$. Then*

$$\frac{\partial\, \mathcal{P}_{G,\ell}(x)}{\partial x} = -\sum_{i=1}^{n} \mathcal{P}_{G_{(i)},\ell}(x).$$

Proof. Observe that $\mathcal{R}_{G,\ell}(x) = \mathcal{P}_{G,\ell}(-x)$. □

Let $\mathcal{D}(G)$ be the terminal distance matrix of G. It can be easily checked that a terminal distance matrix is a submatrix of a graph-theoretical distance matrix of a given graph. The characteristic polynomial $t_G(x) := \det(\mathcal{D}(G) - xI_N)$ of the terminal distance matrix $\mathcal{D}(G)$ of a graph G with N terminal vertices is called the *terminal polynomial* of G. We define the terminal polynomial of a graph G with no terminal vertex as $t_G(x) := 1$.

Observe that in the terminal polynomial of degree m, the coefficient of the term x^{m-1} equals to the trace of the terminal distance matrix, and hence to 0. The leading term equals to $(-x)^N$, where N is the number of terminal vertices of G, and the constant term equals to determinant of the terminal distance matrix of G.

Let v_j be a terminal vertex of a graph G. Let P_{v_j} denote the maximal path in G that starts in v_j and contains (in addition to v_j) only non-terminal vertices of G with valences exactly 2. The generalized Ulam subgraph of G induced by the vertex set $V(G) \setminus V(P_{v_j})$ will be denoted by $G_{[j]}$. As in star-like graphs, we refer to P_{v_j} as j-th ray (with length $V(P_{v_j}) - 1$), see Example 1.

Theorem 3.3 (Terminal Polynomial Theorem)**.** *Let G be a graph with $N > 0$ terminal vertices and $t_G(x)$ its terminal polynomial. Let $G_{[i]}$ denote the graph obtained from G when removing the i-th ray that starts in terminal vertex v_i. Then*

$$\frac{\partial\, t_G(x)}{\partial x} = -\sum_{i=1}^{N} t_{G_{[i]}}(x).$$

Proof. We are given a graph G with $N > 0$ terminal vertices. Let $D(G)$, $\mathcal{D}(G)$ be the graph-theoretical and the terminal distance matrices of G, respectively.

When $N = 1$, $\mathcal{D}(G) = [0]$ and $t_G(x) = \det([-x]) = -x$. Hence $\frac{\partial\, t_G(x)}{\partial x} = -1$. On the other hand, $G_{[1]}$ contains no terminal vertex. Thus, by definition, $t_{G_{[1]}}(x) = 1$, and the theorem holds.

Let us now observe the case when $N > 1$. From G we construct the complete graph K_N, where the i-th terminal vertex $v_i \in V(G)$ is represented by a vertex $u_i \in V(K_N)$. It is easy to see that the Ulam subgraph $K_{N(i)}$ represents the generalized Ulam subgraph $G_{[i]}$.

We label the edges of K_N using labeling

$$\ell(u_i \sim u_j) = D(G)_{i,j}.$$

The labeled adjacency matrix $\mathcal{A}(K_N, \ell)$ gives the characteristic polynomial $\mathcal{P}_{K_N,\ell}(x)$. It can be easilly checked, that

$$A(K_N, \ell) = \mathcal{D}(G),$$

thus the terminal polynomial $t_G(x)$ equals to the characteristic polynomial $\mathcal{P}_{K_N,\ell}(x)$. Similarly, $A(K_{N(i)}, \ell) = \mathcal{D}(G_{[i]}),\ \forall 1 \leq i \leq N$ and hence $t_{G_{[i]}}(x) = \mathcal{P}_{K_{N(i)},\ell}(x)$. Using Corollary 3.2

$$\begin{aligned} \frac{\partial\, t_G(x)}{\partial x} &= \frac{\partial\, \mathcal{P}_{K_N,\ell}(x)}{\partial x} \\ &= -\sum_{i=1}^{N} \mathcal{P}_{K_{N(i)},\ell}(x) \\ &= -\sum_{i=1}^{N} t_{G_{[i]}}(x), \end{aligned}$$

which completes our proof. $\square$

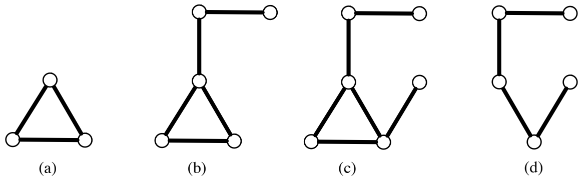


Figure 2: (a) Graph G_a with no terminal vertex. (b) Graph G_b with one terminal vertex. (c) Graph G_c with two terminal vertices. (d) Path G_d on five vertices.

Example 1. *Graphs on Figure 2 have terminal polynomials*

$$\begin{aligned} t_{G_a}(x) &= 1, \\ t_{G_b}(x) &= \det([-x]) = -x, \\ t_{G_c}(x) = t_{G_d}(x) &= \det\left(\begin{bmatrix} 0 & 4 \\ 4 & 0 \end{bmatrix} - x \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) \\ &= \det\left(\begin{bmatrix} -x & 4 \\ 4 & -x \end{bmatrix}\right) = x^2 - 16. \end{aligned}$$

Observe that $G_{b[1]} = G_a$ *and* $G_{d[1]} = G_{d[2]} = K_1$.

Corollary 3.4. *Let* $\mathcal{S} := \mathcal{S}(\{a_1, a_2, \ldots, a_N\})$ *be a star-like graph with* N *rays and* $t_{\mathcal{S}}(x)$ *its terminal polynomial. Let* $\mathcal{S}_{[i]} := \mathcal{S}(\{a_1, \ldots, a_{i-1}, a_{i+1}, \ldots, a_N\})$ *denote the star-like graph obtained from* $\mathcal{S}$ *when removing the* i*-th ray. Then*

$$\frac{\partial\ t_{\mathcal{S}}(x)}{\partial x} = -\sum_{i=1}^{N} t_{\mathcal{S}_{[i]}}(x).$$

Proof. We can, as in Theorem 3.3, define the labeled complete graph K_N on N vertices, using the labeling

$$\ell(u_i \sim u_j) := \begin{cases} a_i + a_j, \ i \neq j, \\ 0, \quad i = j. \end{cases}$$

4 Isoterminal pairs

We say that two different graphs form an *isoterminal pair* of graphs if they have the same terminal polynomial, see Table 1 for the proof that they exist. Since the leading term in the terminal polynomial of a graph with N terminal vertices is $(-x)^N$, both graphs in an isoterminal pair have the same number of terminal vertices.

Let G be a graph and let $k > 0$ be a natural number. With $G(k)$ we label the graph obtained from G by inserting $k-1$ vertices (of valence 2) into each edge of G (by subdividing all edges of G, each $k-1$ times). The following lemma will be used to prove the next theorem.

Lemma 4.1. *Let G be a graph with $N > 0$ terminal vertices, let $k > 1$ be a natural number and let $0 < i \leq N$. Then*

$$G(k)_{[i]} = G_{[i]}(k)$$

Proof. It is easy to see that by inserting $k-1$ vertices into each edge of the i-th ray, we obtain a ray of k-times greater length. $\square$

Theorem 4.2. *Let G be a graph with $N > 0$ terminal vertices and let $k > 1$ be a natural number. Then*

$$t_{G(k)}(x) = k^N \cdot t_G\left(\frac{x}{k}\right).$$

Proof. We will argue by induction on N.

Note that, when $N = 0$, the argument is trivially true. Let us first show that the argument holds for $N = 1$. When $N = 1$, $\mathcal{D}(G) = [0]$ and $t_G(x) = \det([-x]) = -x$ and $t_{G(k)}(x) = k^1 \cdot \left(-\frac{x}{k}\right) = -x$.

Using Theorem 3.3 and induction hypotheses, we may write

$$\begin{aligned}
\frac{\partial\ t_{G(k)}(x)}{\partial x} &= -\sum_{i=1}^{N} t_{G(k)_{[i]}}(x) \\
&= -\sum_{i=1}^{N} t_{G_{[i]}(k)}(x) \\
&= -\sum_{i=1}^{N} k^{N-1} \cdot t_{G_{[i]}}\left(\frac{x}{k}\right) \\
&= -k^{N-1} \cdot \sum_{i=1}^{N} t_{G_{[i]}}\left(\frac{x}{k}\right).
\end{aligned}$$

Let us use a substitution $y = \frac{x}{k}$ and write

$$\begin{aligned}
\int \frac{\partial\ t_{G(k)}(x)}{\partial x} \partial x &= C + \int -k^{N-1} \cdot \sum_{i=1}^{N} t_{G_{[i]}}\left(\frac{x}{k}\right) \partial x \\
&= C + \int -k^{N-1} \cdot \sum_{i=1}^{N} t_{G_{[i]}}(y) \cdot k \cdot \partial y \\
&= C + k^{N} \cdot \int -\sum_{i=1}^{N} t_{G_{[i]}}(y)\ \partial y \\
&= C + k^{N} \cdot \int \frac{\partial\ t_G(y)}{\partial y}\ \partial y
\end{aligned}$$

and

$$t_{G(k)}(x) = C + k^N \cdot t_G(y) = C + k^N \cdot t_G\left(\frac{x}{k}\right),$$

where C is some constant. Since

$$t_{G(k)}(0) = \det(k \cdot \mathcal{D} - 0 \cdot I_n) = k^N \cdot \det(\mathcal{D})$$

and

$$t_G\left(\frac{0}{k}\right) = \det(\mathcal{D} - \left(\frac{0}{k}\right) \cdot I_n) = \det(\mathcal{D}),$$

we can write

$$C = t_{G(k)}(0) - t_G\left(\frac{0}{k}\right) = k^N \cdot \det(\mathcal{D}) - k^N \cdot \det(\mathcal{D}) = 0$$

and

$$t_{G(k)}(x) = k^N \cdot t_G\left(\frac{x}{k}\right).$$

□

Next theorem will prove that for every natural number $N > 0$ we have countably many isoterminal pairs of graphs with exactly N terminal vertices.

Theorem 4.3. *Let G, H be an isoterminal pair of graphs with $N > 0$ terminal vertices and let $k > 1$ be a natural number. Then graphs $G(k)$ and $H(k)$ are an isoterminal pair.*

Proof. Again, let us use a substitution $y = \frac{x}{k}$ and write

$$\begin{aligned} t_{G(k)}(x) &= k^N \cdot t_G\left(\frac{x}{k}\right) \\ &= k^N \cdot t_G(y) \\ &= k^N \cdot t_H(y) \\ &= k^N \cdot t_H\left(\frac{x}{k}\right) \\ &= t_{H(k)}(x). \end{aligned}$$

□

Let G, H be an isoterminal pair of graphs. If there exist a natural number $k > 1$ and an isoterminal pair of graphs G_0, H_0, such that $G = G_0(k)$ and $H = H_0(k)$, we say that the pair G, H is *k-reducible* (and less interesting) pair. Pairs of isoterminal graphs that are not reducible are *ireducible*.

Theorem 4.4. *Let G, H be a k-reducible pair of isoterminal graphs. Then*

$$\gcd_{i \neq j}\{\mathcal{D}(G)_{i,j}, \mathcal{D}(H)_{i,j}\} > 1.$$

Proof. Since G, H are k-reducible, there exist graphs G_0, H_0, such that $G = G_0(k)$ and $H = H_0(k)$. Subdividing all edges of G_0 by inserting $k-1$ vertices into each and every edge of G_0 produces $G_0(k)$ with terminal distance matrix $\mathcal{D}(G_0(k))$. It can be easily checked that $\mathcal{D}(G)_{i,j} = \mathcal{D}(G_0(k))_{i,j} = k \cdot \mathcal{D}(G_0)_{i,j}$. Similar holds for graphs H and H_0. Hence, $\gcd_{i \neq j}\{\mathcal{D}(G)_{i,j}, \mathcal{D}(H)_{i,j}\} = k > 1$. □

Corollary 4.5. *There is countably many isoterminal pairs of star-like graphs.*

Proof. Lemma 4.6 proves that $k-1$ times regularly subdivided star-like graphs are star-like graphs with k times bigger ray lengths. Hence, by Theorem 4.3 and by the fact that an isoterminal pair of star-like graphs exist (see Table 1), we have countably many pairs of isoterminal star-like graphs. □

In general, the existence of a factor $k > 1$ that divides all elements of terminal distance matrices of an isoterminal pair of graphs, does not define the pair to be k-reducible, see Figure 3. On the other hand, this is not the case with star-like graphs.

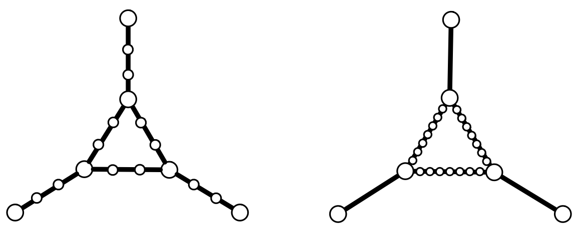


Figure 3: Two ireducible isoterminal graphs with the property that $\gcd_{i \neq j}\{\mathcal{D}(G_a)_{i,j}, \mathcal{D}(G_b)_{i,j}\} = 9$.

Lemma 4.6. *Let $k > 1$ be a natural number. Then*

$$\mathcal{S}(\{a_1, a_2, \ldots, a_N\})(k) = \mathcal{S}(\{k \cdot a_1, k \cdot a_2, \ldots, k \cdot a_N\})$$

Proof. Let $a = \{a_1, a_2, \ldots, a_N\}$ and let $\mathcal{D}(\mathcal{S})$ be the terminal distance matrix of $\mathcal{S}(a)$. Subdividing all edges of $\mathcal{S}(a)$ by inserting $k-1$ vertices into each and every edge of $\mathcal{S}(a)$ produces $\mathcal{S}(k)(a)$ with terminal distance matrix $\mathcal{D}(\mathcal{S}(k))$. It can be easily checked that $\mathcal{D}(\mathcal{S}(k))_{i,j} = k \cdot \mathcal{D}(\mathcal{S})_{i,j}$. By Zaretskii [17], a tree, and hence a star-like graph, is completely determined by its terminal distance matrix. □

Lemma 4.7. *Define $k := \gcd\{a_1, a_2, \ldots, a_N\}$. Then*

$$\mathcal{S}\Big(\Big\{\frac{a_1}{k}, \frac{a_2}{k}, \ldots, \frac{a_N}{k}\Big\}\Big)(k) = \mathcal{S}(\{a_1, a_2, \ldots, a_N\}).$$

Proof. Let $a = \{a_1, a_2, \ldots, a_N\}$. Using Lemma 4.6 we can write

$$\mathcal{S}\left(\frac{a}{k}\right)(k) = \mathcal{S}\left(k \cdot \frac{a}{k}\right) = \mathcal{S}(a).$$

□

Corollary 4.8. *Let $a = \{a_1, a_2, \ldots, a_N\}$, $b = \{b_1, b_2, \ldots, b_N\}$, and let $\mathcal{S}(a)$ and $\mathcal{S}(b)$ be an isoterminal pair of star-like graphs with $k := \gcd\{a_1, \ldots, a_N, b_1, \ldots, b_N\}$. Then $\mathcal{S}(\frac{a}{k})$ and $\mathcal{S}(\frac{b}{k})$ is an isoterminal pair of star-like graphs.*

Proof. Let $A = \{A_1, \ldots, A_N\}$, $B = \{B_1, \ldots, B_N\}$, where $A_i := \frac{a_i}{k}$ and $B_i := \frac{b_i}{k}$. Then, according to Lemma 4.7, $\mathcal{S}(A)(k) = \mathcal{S}(a)$. Hence, $t_{\mathcal{S}(a)}(x) = t_{\mathcal{S}(A)(k)}(x) = k^N \cdot t_{\mathcal{S}(A)}\left(\frac{x}{k}\right) = k^N \cdot t_{\mathcal{S}(A)}(y)$. Similarly, $t_{\mathcal{S}(b)}(x) = k^N \cdot t_{\mathcal{S}(B)}(y)$.

Since $k > 0$ and $t_{\mathcal{S}(a)}(x) = t_{\mathcal{S}(b)}(x)$, $k^N \cdot t_{\mathcal{S}(A)}(y) = k^N \cdot t_{\mathcal{S}(B)}(y)$ and $t_{\mathcal{S}(A)}(y) = t_{\mathcal{S}(B)}(y)$. □

5 Isoterminal pairs of star-like graphs with three rays

Let $a = \{a_1, a_2, \ldots, a_N\}$ and $b = \{b_1, b_2, \ldots, b_N\}$. We can permute the rays of a star-like graph and still obtain the same graph and hence the same terminal polynomial. Thus, we can canonically denote the star-like graph with the lexicographically ordered labeling $\mathcal{S}(a)$, that is, with the labeling, where $1 \leq a_1 \leq a_2 \leq \ldots \leq a_N$. Similarly, we can canonically denote an isoterminal pair with $\mathcal{S}(a)$, $\mathcal{S}(b)$, if and only if a is (lexicographically) smaller than b. See Figure 4 for such a pair.

Let $\mathcal{S}(\{a_1, a_2, a_3\})$ be a three-ray star-like graph. Its terminal distance matrix

$$\mathcal{D}(\mathcal{S}) = \begin{bmatrix} 0 & a_1 + a_2 & a_1 + a_3 \\ a_1 + a_2 & 0 & a_2 + a_3 \\ a_1 + a_3 & a_2 + a_3 & 0 \end{bmatrix}$$

gives the terminal polynomial $t_{\mathcal{S}}(x) = 2(a_1 + a_2)(a_1 + a_3)(a_2 + a_3) + ((a_1 + a_2)^2 + (a_1 + a_3)^2 + (a_2 + a_3)^2)x - x^3$.

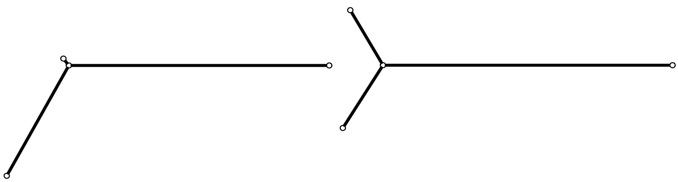


Figure 4: Isoterminal pair of three-ray star-like graphs $\mathcal{S}(\{3, 56, 82\})$ and $\mathcal{S}(\{24, 27, 91\})$ with terminal polynomial $1384140 + 29750x - x^3$.

Let $\mathcal{S}'$ denote the smallest graph (according to canonical notation) of the isoterminal pair $\mathcal{S}_1, \mathcal{S}_2$ of two star-like graphs. With the help of a computer program we calculated all ireducible isoterminal pairs of star-like graphs with three rays, where all ray lengths of the smaller graph $\mathcal{S}'$ (according to the canonical notation) are smaller than 200, see Table 1.

	$\{a,b,c\}$	$\{d,e,f\}$	M
1	{1, 67, 98}	{14, 46, 107}	333
	{1, 67, 168}	{16, 49, 172}	473
	{1, 95, 171}	{41, 45, 183}	536
	{1, 97, 175}	{37, 51, 187}	548
	{1, 98, 177}	{36, 53, 189}	554
	{1, 103, 187}	{33, 61, 199}	584
	{1, 109, 199}	{31, 69, 211}	620
	{1, 119, 137}	{29, 67, 163}	516
	{1, 184, 188}	{43, 97, 236}	749
2	{2, 67, 115}	{16, 47, 122}	369
	{2, 75, 120}	{15, 55, 128}	395
	{2, 98, 169}	{43, 46, 182}	540
	{2, 117, 148}	{13, 93, 162}	535
3	{3, 56, 82}	{24, 27, 91}	283
	{3, 56, 144}	{27, 29, 148}	407
	{3, 72, 97}	{17, 48, 108}	345
	{3, 72, 116}	{17, 51, 124}	383
	{3, 117, 169}	{33, 71, 187}	580
	{3, 119, 153}	{33, 69, 175}	552
	{3, 131, 174}	{14, 108, 187}	617
4	{4, 61, 77}	{26, 28, 89}	285
	{4, 65, 70}	{25, 29, 86}	279
	{4, 183, 191}	{51, 92, 238}	759
	{4, 184, 185}	{52, 89, 235}	749
5	{5, 65, 80}	{26, 32, 93}	301
	{5, 121, 131}	{43, 55, 161}	516
	{5, 121, 167}	{37, 71, 187}	588
	{5, 160, 169}	{16, 125, 194}	669
6	{6, 103, 127}	{19, 76, 142}	473
	{6, 178, 199}	{58, 87, 241}	769
7	{7, 66, 103}	{31, 34, 112}	353
	{7, 66, 179}	{34, 36, 183}	505
	{7, 88, 92}	{23, 53, 112}	375
	{7, 121, 169}	{43, 67, 189}	596
	{7, 123, 141}	{51, 53, 169}	544
	{7, 141, 149}	{39, 77, 183}	596
8	{8, 69, 117}	{30, 40, 125}	389
	{8, 100, 103}	{23, 64, 125}	423
	{8, 145, 163}	{20, 113, 184}	633
9	{9, 129, 151}	{51, 61, 179}	580
	{9, 149, 195}	{39, 97, 219}	708

	$\{a,b,c\}$	$\{d,e,f\}$	M
10	{10, 92, 111}	{27, 60, 127}	427
11	{11, 88, 97}	{32, 49, 116}	393
	{11, 149, 157}	{47, 79, 193}	636
12	{12, 88, 107}	{33, 52, 123}	415
	{12, 125, 162}	{26, 97, 177}	599
13	{13, 82, 122}	{38, 47, 133}	435
	{13, 92, 117}	{33, 58, 132}	445
	{13, 127, 132}	{28, 88, 157}	545
	{13, 131, 191}	{61, 65, 211}	672
	{13, 159, 177}	{47, 93, 211}	700
	{13, 169, 172}	{46, 97, 213}	710
14	{14, 88, 121}	{37, 53, 134}	447
	{14, 148, 151}	{28, 107, 179}	627
15	{15, 161, 181}	{51, 93, 215}	716
16	{16, 94, 137}	{38, 61, 149}	495
	{16, 182, 193}	{29, 142, 221}	783
17	{17, 94, 186}	{39, 66, 193}	595
	{17, 126, 138}	{34, 87, 161}	563
	{17, 136, 193}	{32, 109, 206}	693
21	{21, 169, 179}	{71, 81, 219}	740
	{21, 175, 177}	{67, 87, 221}	748
23	{23, 109, 166}	{47, 74, 178}	597
	{23, 122, 131}	{47, 74, 156}	553
	{23, 159, 186}	{39, 122, 208}	737
	{23, 161, 182}	{39, 122, 206}	733
25	{25, 107, 192}	{52, 72, 201}	649
	{25, 111, 144}	{60, 60, 161}	561
26	{26, 106, 181}	{61, 62, 191}	627
	{26, 117, 138}	{61, 62, 159}	563
28	{28, 143, 180}	{48, 105, 199}	703
31	{31, 124, 182}	{59, 83, 196}	675
	{31, 138, 140}	{63, 76, 171}	619
36	{36, 173, 189}	{57, 124, 218}	797
37	{37, 138, 172}	{73, 82, 193}	695
39	{39, 138, 191}	{74, 87, 208}	737
	{39, 148, 186}	{68, 99, 207}	747
	{39, 162, 196}	{63, 116, 219}	795
42	{42, 179, 184}	{67, 120, 219}	811
44	{44, 165, 171}	{80, 96, 205}	761
46	{46, 172, 185}	{77, 110, 217}	807
54	{54, 184, 193}	{94, 109, 229}	863

Table 1: All irreducible pairs of isoterminal star-like graphs $\mathcal{S}(\{a,b,c\}), \mathcal{S}(\{d,e,f\})$ with three rays in canonical notation, where the ray lengths of the smallest graph $\mathcal{S}(\{a,b,c\})$ (according to the canonical notation) are smaller than 200 and where $M = a+b+c+d+e+f$.

The isoterminal pair $\mathcal{S}(\{11,88,97\}), \mathcal{S}(\{32,49,116\})$ of Randić and Kleiner [13] is listed in Table 1. Note that rays in one graph can be of the same length, for example look at pair $\mathcal{S}(\{25,111,144\}), \mathcal{S}(\{60,60,161\})$ in Table 1. Moreover, in all cases $a < d$, $b > e$ and $c < f$. Isoterminal pairs of Table 1 have different terminal matrices but the same terminal polynomial while graphs on Figure 5 have the same terminal matrix and consequently the same polynomial.

Lemma 5.1. *Let $\mathcal{S}(\{a, b, c\})$, $\mathcal{S}(\{d, e, f\})$ be an isoterminal pair of star-like graphs with 3 rays. Then $a, b, c \notin \{d, e, f\}$.*

Proof. Without loss of generality (because of the symmetry) we may assume that $a = d$. Then we can write two equations

$$(a + b)(a + c)(b + c) = (a + e)(a + f)(e + f)$$

and

$$(a + b)^2 + (a + c)^2 + (b + c)^2 = (a + e)^2 + (a + f)^2 + (e + f)^2.$$

With simple arithmetic operations we can transform them into

$$2a(b + c - e - f) - e^2 - f^2 - (e + f)^2 + b^2 + c^2 + (b + c)^2) = 0$$

and

$$a^2(b + c - e - f) + a((b + c)^2 - (e + f)^2) + bc(b + c) - ef(e + f) = 0.$$

First, let us assume that $b + c - e - f \neq 0$. Then we can write

$$a = \frac{e^2 + f^2 + (e + f)^2 - b^2 - c^2 - (b + c)^2)}{2(b + c - e - f)}$$

and insert it into the second equation. The simplified second equation now becomes

$$\frac{(b - e)(c - e)(b - f)(c - f)}{b + c - e - f} = 0$$

and the four solutions are $e = b$, $e = c$, $f = b$ and $f = c$. Considering each solution and the first equation, we obtain the solution for the other variable and hence

- $e = b,\ f = -(a + b + c)$,
- $e = c,\ f = -(a + b + c)$,
- $e = -(a + b + c),\ f = b$,
- $e = -(a + b + c),\ f = c$.

Now, let us assume that $b + c - e - f = 0$. Then we can write $f = b + c - e$ and using it in the first equation would yield the equation $2(b - e)(c - e) = 0$. We obtain another two solutions

- $e = b,\ f = c$,
- $e = c,\ f = b$.

The first four solutions have negative ray lengths, thus do not represent valid star-like graphs. The other two solutions determine the same graph, thus we obtain a trivial isoterminal pair of star-like graphs. $\square$

Since there are countably many isoterminal pairs of star-like graphs with three rays, it makes sence to find the smallest one (according to some canonical notation).

Proposition 5.2. *Let $\mathcal{S}(\{a_1, a_2, a_3\}), \mathcal{S}(\{b_1, b_2, b_3\})$ be an isoterminal pair of star-like graphs with 3 rays, with the smallest sum $M := a_1 + a_2 + a_3 + b_1 + b_2 + b_3$. Then there is exactly one such pair $\mathcal{S}(\{4, 65, 70\})$, $\mathcal{S}(\{25, 29, 86\})$ and $M = 279$.*

Proof. Let $\mathcal{S}(\{a_1, a_2, a_3\})$ and $\mathcal{S}(\{b_1, b_2, b_3\})$ be an isoterminal pair of star-like graphs in canonical notation. Define $M := a_1 + a_2 + a_3 + b_1 + b_2 + b_3$ and $N := \prod_{i<j}(a_i + a_j)$.

Then $1 \le a_1 \le \lceil \frac{M}{6} \rceil$, $a_1 \le a_2 \le \lceil \frac{M-4a_1}{2} \rceil$ and $a_2 \le a_3 \le M - 4a_1 - a_2$. On the other hand $(b_1 + b_2)$ divides N and $(b_1 + b_2) \le \sqrt[3]{N}$. Define $\mathcal{F} := \{f \mid f \text{ divides } N\}$. Then $b_2, b_3 \in \{f - b_1 \mid f \in \mathcal{F}\}$. Moreover, $a_1 \le b_1 \le \lceil \frac{\sqrt[3]{N}}{2} \rceil$, $b_1 \le b_2 \le \sqrt[3]{N} - b_1$ and $b_2 \le b_3$. The result was obtained with the help of a computer program, calculating all isoterminal pairs with ray-lengths within allowed range. The minimal sum $\sum_{i=1}^{3}(a_i + b_i) = 279$ determines the smallest isoterminal pair $\mathcal{S}(\{4, 65, 70\})$, $\mathcal{S}(\{25, 29, 86\})$. $\square$

6 Conclusions

In the paper we presented the theory about terminal polynomials and proved the Clarke-type theorem for terminal polynomials. We observed star-like graphs and their terminal polynomials. We calculated all ireducible isoterminal polynomials of star-like graphs with three rays where the ray lengths of the smaller graph in the pair are smaller than 200.

It would be interesting to calculate minimal star-like graphs with more that three rays, especially with rays up to 20, see [15].

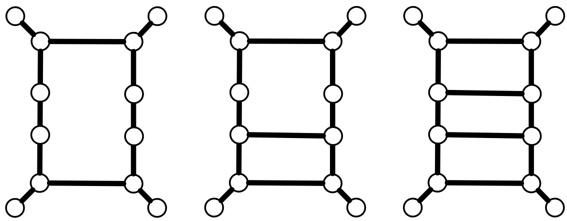
We noticed that sometimes isoterminal pairs can be obtained from a given isoterminal pair with inserting vertices (inserting the same number of vertices in corresponding rays) in both graphs that form the given isoterminal pair, see Table 2 for more details. The question "Given an isoterminal pair, what is the minimum number of vertices that must be added to both graphs, to obtain another isoterminal pair?" still remains open.

$\{a, b, c\}$	$\{d, e, f\}$	$\{a', b', c'\}$	$\{d', e', f'\}$	$\{i, j, k\}$
{4, 61, 77}	{26, 28, 89}	{16, 94, 137}	{38, 61, 149}	{12, 33, 60}
{4, 65, 70}	{25, 29, 68}	{12, 88, 107}	{33, 52, 123}	{8, 23, 37}
{25, 111, 144}	{60, 60, 161}	{39, 138, 191}	{74, 87, 208}	{14, 27, 47}

Table 2: Isoterminal pairs $\mathcal{S}(\{a, b, c\})$, $\mathcal{S}(\{d, e, f\})$ and $\mathcal{S}(\{a', b', c'\})$, $\mathcal{S}(\{d', e', f'\})$, with the property that there exist a triple $\{i, j, k\}$, $i, j, k \geq 0$, such that $\{a', b', c'\} = \{a + i, b + j, c + k\}$ and $\{d', e', f'\} = \{d + i, e + j, f + k\}$.

By connecting two non-terminal vertices $u, v \in V(G)$ of a given graph G, with a path that is longer than the graph-theoretical distance between the vertices u and v, one does not change the terminal matrix. Hence, we can construct infinite number of graphs that are isoterminal to G, see an example of an isoterminal triple on Figure 5. But such a construction yields a cycle, thus it can not be used with star-like graphs;

therefore, there is another question to be answered, namely, "For a given natural number $n > 2$ is there an isoterminal n-tuple of star-like graphs?".



(a) (b) (c)

Figure 5: Non-isomorphic graphs having the same number of vertices and the same terminal polynomial.

Remark that some authors (see for example [6]) called the polynomial $\mathcal{R}_{G,1}(x)$, defined in Section 2, "the characteristic polynomial" of the graph. Since our notation is now widely used, the reader should be aware of that, while using our results with the older papers on this topic.

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