CROATICA CHEMICA ACTA
CCACAA, ISSN 0011-1643, e-ISSN 1334-417X
Croat. Chem. Acta **82** (3) (2009) 679–684.
CCA-3360

Original Scientific Paper

On the Calculation of the Terminal Polynomial of a Star-like Graph

Boris Horvat

IMFM, University of Ljubljana, Jadranska 19, Ljubljana, Slovenia
(*E-mail: boris.horvat@fmf.uni-lj.si*)

RECEIVED MAY 5, 2008; REVISED AUGUST 7, 2008; ACCEPTED AUGUST 9, 2008

Abstract. The terminal matrix is the distance matrix between all pairs of valence one vertices of a given graph and the terminal polynomial is the characteristic polynomial of the terminal matrix. Star-like graphs are connected graphs with at most one vertex of degree $d \geq 3$. The recursive formula that calculates the terminal polynomial of a star-like graph is given. Particularly, the formula that calculates the constant term in the terminal polynomial is given in closed form.

Keywords: terminal polynomial, terminal polynomial theorem, star-like graph, Clarke Theorem

INTRODUCTION

Informally, star graphs are connected graphs with at most one vertex of degree $d \geq 2$, while star-like graphs are connected graphs with at most one vertex (sometimes called the hub vertex) of degree $d \geq 3$ (and with other vertices with degrees less or equal two). A path in a star-like graph S, which connects the hub vertex of S with a vertex of valence one (also called terminal vertex) of S, is called a ray. By removing a ray from a star-like graph, a smaller star-like graph (also called ray factor) is obtained.

Recently, terminal polynomials of graphs with at least one vertex of valence one have been considered[1] and it was proven that the so-called Clarke-type property[2] also holds for terminal polynomials. Gutman and co-workers studied their mathematical and spectral properties.[4–7] Even though a tree (and hence a star-like graph) is completely defined by its terminal distance matrix,[8] this is not the case with the terminal polynomial.[1,8] There exist star-like graphs with different terminal distance matrices and with the same terminal polynomial (such graphs will be called isoterminal graphs).

Star-like graphs have been considered for construction of graphical representation of proteins,[3] so that their invariants can serve as numerical descriptors for characterization of proteins and facilitate computer-based comparative study of proteins. Among relatively simple invariants belong the eigenvalues of the terminal matrix, and in view of potential use of eigenvalues of the terminal polynomial as protein descriptors, it is of considerable interest to investigate the existence of pairs of non-isomorphic star-like graphs, having from three rays to 20 rays (in view that proteins are build from at most 20 different natural amino acids).The calculation of all isoterminal pairs of star-like graphs with three rays, where the smallest graph in the pair contained at most 201 vertices, has been recently done.[1] In the same paper was shown, that countably many isoterminal pairs of star-like graphs exist. All isoterminal pairs of star-like graphs that are presently known have exactly three rays.[1,9]

Constructing a star-like graph from star-like graphs with smaller number of rays can help obtaining additional isoterminal pairs of (bigger) star-like graphs. Thus, a formula that can be used to calculate the terminal polynomial of a given star-like graph, using the terminal polynomials of its ray factors, is also of interest. In this paper, the recursive formula that calculates the terminal polynomial of a star-like graph is given. Particularly, the formula that calculates the constant term in the terminal polynomial is given in closed form.

CALCULATING THE TERMINAL POLYNOMIAL OF A STAR-LIKE GRAPH

All graphs in this paper are considered to be finite, undirected and connected graphs, with no loops or multiple edges. 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 $\mathrm{S}(a)$ with n rays is a graph with vertex set $V(S(a)) = \{u\} \cup \{v_{i,j}, 1 \le i \le n, 1 \le j \le a_i\}$ and edge set $E(S(a)) = \{u \sim v_{i,1}, 1 \le i \le n\} \cup \{v_{i,j} \sim v_{i,j-1}, 1 \le i \le n, 2 \le j \le a_i\}$. Thus $|V(S(a))| = 1 + \sum_{j=1}^{n} a_j$ and $|E(S(a))| = \sum_{j=1}^{n} a_j$. The induced subgraph of $S(a)$ on the vertex set $\{v_{i,j}, 1 \le j \le a_i\}$ will be called the *i*-th ray. A star graph is a star-like graph with all rays of length one. Remark, that a path on at least two vertices is a (degenerate and thus less interesting) star-like graph.

Let G be a graph. Define $\boldsymbol{D}$(G) to be the graph-theoretical distance matrix of G and let $\boldsymbol{T}$(G) be the graph-theoretical distance matrix of distances between all pairs of valence one vertices (or terminal vertices) of G. We refer to $\boldsymbol{T}$(G) as the terminal (distance) matrix of G. Observe that the terminal matrix is non-negative, symmetric, real matrix with zero trace and real eigenvalues. The properties of matrices with similar structure have been recently observed.[10] It is known that every tree is completely defined by its terminal distance matrix.[8] Moreover, the terminal matrix of a star-like graph is determined by its first row and any other non-diagonal element. The element in *i*-th row and *j*-th column of a matrix $\boldsymbol{M}$ will be denoted by $\boldsymbol{M}_{i,j}$.

Let G be a graph with $n > 0$ terminal vertices and let $\boldsymbol{I}_n$ be the $n \times n$ identity matrix. The characteristic polynomial

$$t_{\mathrm{G}}(x) = \det(\boldsymbol{T}(\mathrm{G}) - x\boldsymbol{I}_n)$$

of the terminal matrix $\boldsymbol{T}$(G) of G, is called the terminal polynomial of G. We define the terminal polynomial of a graph G^* with no terminal vertex as $t_{\mathrm{G}^*}(x) := 1$. 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. The following terminal polynomial theorem (Clarke-type[2] theorem for terminal polynomials) has been recently proved.[1]

Theorem 1. (Terminal polynomial theorem) Let G be a graph with $n > 0$ terminal vertices, let v_i be its *i*-th terminal vertex and let $t_{\mathrm{G}}(x)$ be its terminal polynomial. Denote the graph obtained from G, when removing the *i*-th ray that starts in terminal vertex v_i, by $\mathrm{G}_{[i]}$. Then

$$\frac{\partial\, t_{\mathrm{G}}(x)}{\partial x} = -\sum_{i=1}^{n} t_{\mathrm{G}[i]}(x),$$

where the terminal polynomial of a graph with no terminal vertex is one.

By the above expression, the terminal polynomial has all terms but the constant term defined and since we are observing finite graphs (and hence finite sums), we can write

$$t_{\mathrm{G}}(x) = -\sum_{i=1}^{n} \int t_{\mathrm{G}_{[i]}}(x)dx + C_{\mathrm{G}},$$

where again, the terminal polynomial of a graph with no terminal vertex is one. The constant term C_{G} equals to $t_{\mathrm{G}}(0)$ and hence $C_{\mathrm{G}} = \det(\boldsymbol{T}(\mathrm{G}))$. What remains is to calculate the determinant of the terminal matrix of G.

When the terminal polynomial $t_{\mathrm{S}}(x)$ of a star-like graph S is considered, the terminal matrix $\boldsymbol{T}$(S) is defined as

$$\boldsymbol{T}(\mathrm{S})_{i,j} = \begin{cases} 0, & i = j, \\ a_i + a_j, & i \ne j. \end{cases}$$

The following theorem (the main theorem of this paper) will be proved in Section 3.

Theorem 2. Let S be a star-like graph with $n > 2$ terminal vertices and ray lengths $a_1, a_2, \ldots, a_n$. Let $\boldsymbol{T}$(S) be the terminal matrix of S. Then

$$\det(\boldsymbol{T}(\mathrm{S})) = (-2)^{n-2} \prod_{i=1}^{n} a_i \left((n-2)^2 - \sum_{i=1}^{n} \frac{1}{a_i} \sum_{j=1}^{n} a_j \right).$$

Now we can write the recursive formula for calculating the terminal polynomial of a star-like graph.

Corollary 3. Let S be a star-like graph with $n > 2$ terminal vertices and ray lengths $a_1, a_2, \ldots, a_n$. Let v_i be the *i*-th terminal vertex of S and let $\mathrm{S}_{[i]}$ denote the graph obtained from S when removing the *i*-th ray that starts in terminal vertex v_i. Then, the terminal polynomial of S can be recursively calculated as

$$t_{\mathrm{S}}(x) = -\sum_{i=1}^{n} \int t_{\mathrm{S}_{[i]}}(x)dx + (-2)^{n-2} \prod_{i=1}^{n} a_i \left((n-2)^2 - \sum_{i=1}^{n} \frac{1}{a_i} \sum_{j=1}^{n} a_j \right),$$

where the terminal polynomial of a star-like graph with exactly two terminal vertices is $x^2 - (a_1 + a_2)^2$.

The following example illustrates the use of Corollary 3.

Example. Let $\mathrm{S}_a = \mathrm{S}(\{a_1, a_2, a_3\})$, $\mathrm{S}_b = \mathrm{S}(\{a_1, a_2, a_4\})$, $\mathrm{S}_c = \mathrm{S}(\{a_1, a_3, a_4\})$, $\mathrm{S}_d = \mathrm{S}(\{a_2, a_3, a_4\})$ and $\mathrm{S}_e = \mathrm{S}(\{a_1, a_2, a_3, a_4\})$ be star-like graphs as defined on Figure 1.

Their terminal polynomials are

$$t_{\mathrm{S}_a}(x) = 2(a_1 + a_2)(a_1 + a_3)(a_2 + a_3) + ((a_1 + a_2)^2 + (a_1 + a_3)^2 + (a_2 + a_3)^2)x - x^3,$$

$$t_{\mathrm{S}_b}(x) = 2(a_1 + a_2)(a_1 + a_4)(a_2 + a_4) + ((a_1 + a_2)^2 + (a_1 + a_4)^2 + (a_2 + a_4)^2)x - x^3,$$

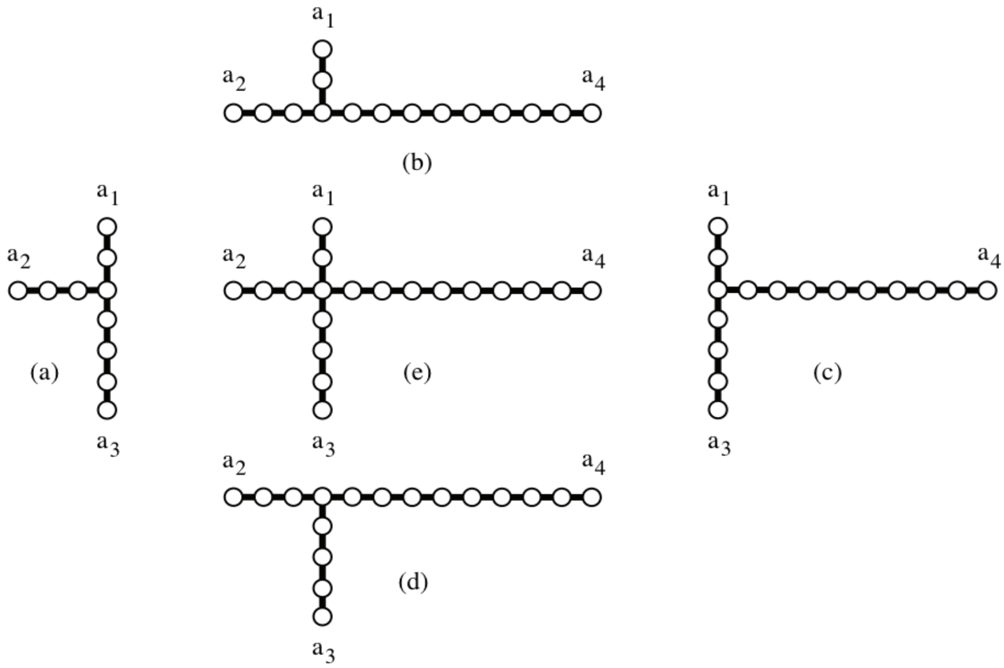

Figure 1. Star-like graphs S_a, S_b, S_c and S_d are obtained from star-like graph S_e by ray deleting.

$$t_{S_c}(x) = 2(a_1+a_3)(a_1+a_4)(a_3+a_4) + ((a_1+a_3)^2+(a_1+a_4)^2+(a_3+a_4)^2)x - x^3,$$

$$t_{S_d}(x) = 2(a_2+a_3)(a_2+a_4)(a_3+a_4) + ((a_2+a_3)^2+(a_2+a_4)^2+(a_3+a_4)^2)x - x^3$$

and

$$\begin{aligned} t_{S_e}(x) = {} & -4(a_1a_2a_3(a_1+a_2+a_3)+a_1a_2a_4(a_1+a_2+a_4)+ \\ & a_1a_3a_4(a_1+a_3+a_4)+a_2a_3a_4(a_2+a_3+a_4) - \\ & 4x(a_1^2a_2+a_1a_2^2+a_1^2a_3+a_1a_2a_3+a_2^2a_3+a_1a_3^2+ \\ & a_2a_3^2+a_1^2a_4+a_1a_2a_4+a_2^2a_4+a_1a_3a_4+a_2a_3a_4+ \\ & a_3^2a_4+a_1a_4^2+a_2a_4^2+a_3a_4^2) - x^2(3a_1^2+2a_1a_2+ \\ & 3a_2^2+2a_1a_3+2a_2a_3+3a_3^2+2a_1a_4+2a_2a_4+ \\ & 2a_3a_4+3a_4^2)+x^4. \end{aligned}$$

Using Theorem 2, we can write

$$\det(T(S_e)) = -4x(a_1^2a_2+a_1a_2^2+a_1^2a_3+a_1a_2a_3+ a_2^2a_3+a_1a_3^2+a_2a_3^2+a_1^2a_4).$$

By integrating the sum of all terminal polynomials of the subgraphs on three rays $\int (t_{S_a}(x)+t_{S_b}(x)+t_{S_c}(x)+t_{S_d}(x))\,dx$, multiplying the result by –1 and adding the constant term $\det(\boldsymbol{T}(S_e))$ to it, the terminal polynomial $t_{S_e}(x)$ is obtained. Note that $t_{S_a}(x)$, $t_{S_b}(x)$, $t_{S_c}(x)$ and $t_{S_d}(x)$ were obtained in a similar way from their subgraphs and corresponding terminal matrices.

PROOF OF THEOREM 2

Define the following expressions

$$\boldsymbol{P} := \prod_{k=1}^{n} a_k, \quad \boldsymbol{R} := \sum_{k=1}^{n} \frac{1}{a_k}, \quad \boldsymbol{W} := \sum_{k=1}^{n} a_k,$$

which will be used throughout this section.

Lemma 4. Let G be a weighted tree on $n+1$ vertices with edge weights $a_1, a_2, \ldots, a_n$, and let $\boldsymbol{D}$ be the distance matrix of G. Then,

$$\det(\boldsymbol{D}) = (-1)^n\, 2^{n-1} \boldsymbol{PW}.$$

Proof. Use Corollary 2.5 from Ref. 1, observing a tree with $n+1$ vertices.

The following Sherman-Morrison formula[11] is well known. In the present form it appeared in Ref. 12.

Lemma 5. Let $\boldsymbol{G}$ and $\boldsymbol{G}+\boldsymbol{H}$ be nonsingular matrices where $\boldsymbol{H}$ is a matrix of rank one. Let $g = \mathrm{tr}(\boldsymbol{HG}^{-1})$ be the trace of the matrix $\boldsymbol{HG}^{-1}$. Then $g \neq -1$ and

$$\boldsymbol{G}^{-1} - \frac{1}{1+g}\boldsymbol{G}^{-1}\boldsymbol{HG}^{-1}$$

is the inverse of $\boldsymbol{G}+\boldsymbol{H}$.

In the proof of our main result, the inverse of the terminal matrix will be needed.

Theorem 6. Let S be a star graph on $n > 2$ terminal vertices with edge weights $a_1, a_2, \ldots, a_n$ and let $\boldsymbol{A}$ be the terminal matrix of S. Then

$$\boldsymbol{A}_{i,j}^{-1} = \begin{cases} \dfrac{1}{2(n-2)}\left(\dfrac{3-n}{a_j} - \boldsymbol{E}_{i,j}\right), i = j, \\ \dfrac{1}{2(n-2)}\left(\dfrac{1}{a_j} - \boldsymbol{E}_{i,j}\right), i \neq j, \end{cases}$$

where

$$\boldsymbol{E}_{i,j} := \frac{1}{\boldsymbol{RW} - (n-2)^2}\left(\frac{(n-2)^2}{a_i} - \frac{(n-2)\boldsymbol{W}}{a_i a_j} - (n-2)\boldsymbol{R} + \frac{\boldsymbol{RW}}{a_j}\right).$$

Proof. As before, observe that

$$\boldsymbol{A}_{i,j} = \begin{cases} 0, \ i = j, \\ a_i + a_j, i \neq j. \end{cases}$$

Define $\boldsymbol{H}_{i,j} := a_j$ and $\boldsymbol{G} := \boldsymbol{A} - \boldsymbol{H}$. It is easy to see that rank of $\boldsymbol{H}$ is one, and that

$$\boldsymbol{G}_{i,j} = \begin{cases} -a_i, i = j, \\ a_i, i \neq j. \end{cases}$$

Since a_i, $1 \leq i \leq n$, are positive natural numbers, $\boldsymbol{G}$ is nonsingular and matrix elements of its inverse can be shown to be

$$\boldsymbol{G}_{i,j}^{-1} = \begin{cases} \dfrac{1}{2(n-2)}\dfrac{3-n}{a_j}, i = j, \\ \dfrac{1}{2(n-2)}\dfrac{1}{a_j}, i \neq j. \end{cases}$$

Furthermore,

$$(\boldsymbol{HG}^{-1})_{i,j} = -\frac{1}{2} + \frac{\boldsymbol{W}}{2(n-2)a_j} \text{ and}$$

$$g = \mathrm{tr}(\boldsymbol{HG}^{-1}) = -\frac{n}{2} + \frac{\boldsymbol{RW}}{2(n-2)}. \text{ Then}$$

$$(\boldsymbol{G}^{-1}\boldsymbol{HG}^{-1})_{i,j} = \frac{1}{4(n-2)^2}\left(\frac{2-n}{a_i} + \boldsymbol{R}\right)\left(2 - n + \frac{\boldsymbol{W}}{a_j}\right).$$

We prove our theorem by using Lemma 5 with $\boldsymbol{G}$ and $\boldsymbol{H}$.

Lemma 7. Let S be a star graph on $n > 2$ terminal vertices with edge weights $a_1, a_2, \ldots, a_n$, and let $\boldsymbol{A}$ be the terminal matrix of S. Then,

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_i a_j \boldsymbol{A}_{i,j}^{-1} = \frac{2\boldsymbol{W}}{\boldsymbol{RW} - (n-2)^2}.$$

Proof. Using the same notation as in Theorem 6, we can write

$$\sum_{j=1}^{n} a_j \boldsymbol{A}_{i,j}^{-1} = \frac{1}{(n-2)} - \frac{1}{2(n-2)}\frac{1}{\boldsymbol{RW} - (n-2)^2}\left(-\frac{2(n-2)\boldsymbol{W}}{a_i} + 2\boldsymbol{RW}\right)$$

and

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_i a_j \boldsymbol{A}_{i,j}^{-1} = \sum_{i=1}^{n} a_i \sum_{j=1}^{n} a_j \boldsymbol{A}_{i,j}^{-1} = \frac{2\boldsymbol{W}}{\boldsymbol{RW} - (n-2)^2}.$$

Hence the result holds.

Now we are able to prove the following result concerning the determinant of the terminal matrix for a star graph on at least three terminal vertices.

Proposition 8. Let S be a star graph on $n > 2$ terminal vertices with edge weights $a_1, a_2, \ldots, a_n$, and let $\boldsymbol{A}$ be the terminal matrix of S. Then,

$$\det(\boldsymbol{A}) = (-2)^{n-2}\boldsymbol{P}\left((n-2)^2 - \boldsymbol{RW}\right).$$

Proof. Let $\boldsymbol{M}$ be the distance matrix of S. We can reorder (if necessary) the vertices of S, such that the rod vertex with the valence greater than two is labeled with v_{n+1}. Hence the other vertices are labeled with v_i, where $1 \leq i \leq n$. It is easy to see that the terminal matrix $\boldsymbol{A} = \boldsymbol{M}(n+1; n+1)$ is the principal upper-left square submatrix of dimension n of matrix $\boldsymbol{M}$, formed by removing the $(n+1)$-th row and the $(n+1)$-th column from $\boldsymbol{M}$. Thus,

$$\boldsymbol{M} = \begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix},$$

where $\boldsymbol{B}^T = (a_1, a_2, \ldots, a_n)$, $\boldsymbol{C} = (a_1, a_2, \ldots, a_n)$ and $\boldsymbol{D} = 0$. The well-known equation

$$\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix} = \begin{pmatrix} \boldsymbol{A} & 0 \\ \boldsymbol{C} & 1 \end{pmatrix}\begin{pmatrix} 1 & \boldsymbol{A}^{-1}\boldsymbol{B} \\ 0 & \boldsymbol{D} - \boldsymbol{CA}^{-1}\boldsymbol{B} \end{pmatrix}$$

gives

$$\det\left(\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix}\right) = \det(\boldsymbol{A})\det(\boldsymbol{D} - \boldsymbol{CA}^{-1}\boldsymbol{B}),$$

hence

$$\det(\boldsymbol{M}) = \det(\boldsymbol{A})\det(0 - \boldsymbol{CA}^{-1}\boldsymbol{B}) = -\det(\boldsymbol{A})\det(\boldsymbol{CA}^{-1}\boldsymbol{B})$$

and

$$\det(\boldsymbol{A}) = -\det(\boldsymbol{M})\det(\boldsymbol{CA}^{-1}\boldsymbol{B}).$$

By Lemma 7

$$\det(\boldsymbol{C}\boldsymbol{A}^{-1}\boldsymbol{B}) = \sum_{i=1}^{n}\sum_{j=1}^{n} a_i a_j \boldsymbol{A}_{i,j}^{-1} = \frac{2\boldsymbol{W}}{\boldsymbol{R}\boldsymbol{W} - (n-2)^2}.$$

Since star graph S is a weighted tree on $n+1$ vertices we can (following Lemma 4) write

$$\det(\boldsymbol{A}) = -\frac{\det(\boldsymbol{M})}{\det(\boldsymbol{C}\boldsymbol{A}^{-1}\boldsymbol{B})} = (-2)^{n-2}\,\boldsymbol{P}\Big((n-2)^2 - \boldsymbol{R}\boldsymbol{W}\Big),$$

which proves our proposition.

Finally, we can prove our main result.

Proof. (Proof of the Theorem 2) From a star-like graph S with $n > 2$ terminal vertices, the star graph S^* with *n* terminal vertices can be constructed, such that each ray of S is represented by the weighted edge in S^*; the weight of the edge being the corresponding ray's length. The terminal matrices of star-like graph S and the corresponding star graph S^* are equal. Thus, we can use Proposition 8 to complete our proof.

To complete the result concerning the constant term of the terminal polynomial of a star-like graph with less than three terminal vertices, we state the obvious cases in the following remark.

Remark. Let S be a star-like graph with 2 terminal vertices and let $\{a_1, a_2\}$ be its ray lengths. The terminal distance matrix equals to

$$\boldsymbol{R}(\mathrm{S}) = \begin{pmatrix} 0 & a_1 + a_2 \\ a_1 + a_2 & 0 \end{pmatrix}$$

and its determinant to $\det(\boldsymbol{T}(\mathrm{S})) = -(a_1 + a_2)^2$. When S is a star-like graph with only one terminal vertex, its terminal distance matrix equals to $\boldsymbol{T}(\mathrm{S}) = \begin{pmatrix} 0 \end{pmatrix}$ and its determinant to $\det(\boldsymbol{T}(\mathrm{S})) = 0$. By a definition, the constant term of the terminal polynomial of a graph with no terminal vertices equals to one.

CONCLUSIONS

Let us finish with some open problems. Since star-like graphs are used for a visual representation of proteins, graphs with up to 20 rays are being studied. As already said, star-like graphs on three rays with the sum of ray lengths smaller than 200, having the same terminal spectra have been observed recently.[1] Motivated by these results, one can formulate interesting problems: »Are there pairs (triples, *etc*.) of star-like graphs with four, five, ... terminal vertices that are isoterminal?«, »Find the pair of isoterminal star-like graphs with four, five, ... rays having the smallest number of vertices (contained in both graphs in the pair).«, »Are there finitely many isoterminal pairs of star-like graphs with four, five, ... rays?« and »Is there an isoterminal pair of star-like graphs with the property that each of ray factors of the first graph in the pair is an isoterminal mate of a ray factor of the second graph in the pair?«.

Acknowledgements. The author would like to thank professor Milan Randić for his comments and suggestions. Research was supported in part by grants P1-0294, J1-6062 and L1-7230 from Ministry of high education, science and technology of the Republic of Slovenia.

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SAŽETAK

O računanju terminalnog polinoma zvijezdolikog grafa

Boris Horvat

IMFM, University of Ljubljana, Jadranska 19, Ljubljana, Slovenia

Terminalnom matricom naziva se matrica udaljenosti između čvorova grafa koji imaju valenciju jedan, a terminalni polinom je naziv za karakteristični polinom terminalne matrice. Zvijezdoliki grafovi su povezani grafovi s najviše jednim čvorom stupnja $d \geq 3$. U radu je prikazana rekurzivna formula za račun terminalnog polinoma zvijezdolikog grafa. Posebno je za konstantni član terminalnog polinoma izvedena formula u zatvorenom obliku.