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A complete solution to a conjecture on the β-polynomials of graphs

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In 1990, Gutman and Mizoguchi conjectured that all roots of the β-polynomial $\beta(G, C, x)$ of a graph G are real. Since then, there has been some literature intending to solve this conjecture. However, in all existing literature, only classes of graphs were found to show that the conjecture is true; for example, monocyclic graphs, bicyclic graphs, graphs such that no two circuits share a common edge, graphs without 3-matchings, etc, supporting the conjecture in some sense. Yet, no complete solution has been given. In this paper, we show that the conjecture is true for all graphs, and therefore completely solve this conjecture.

KEY WORDS: matching polynomial, β-polynomial, path tree

1. Introduction

Throughout the paper, all graphs are finite and simple, and a circuit C of a graph G means a connected subgraph of G such that every vertex of C has degree 2. For notations and terminology not defined here, we refer to [1,2]. Let $V(G)$ and $E(G)$ denote the set of vertices and the set of edges of a graph G, respectively.

Let G be a graph with n vertices. Denote by $m(G, k)$ the number of k-matchings of G. The *matching polynomial* of G is defined by

$$\alpha(G, x) = \sum_{k\geqslant 0}(-1)^k m(G, k)x^{n-2k},$$

where $m(G, 0) = 1$. Matching polynomials are extensively studied in chemical graph theory. It is well-known that all roots of a matching polynomial are real, see [2,3].

Let H be a subgraph of G. We denote by $G\backslash H$ the subgraph of G obtained by deleting the vertices of H from G. Let uv be an edge of G. We denote by $G - uv$ the

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graph obtained by deleting the edge uv from G. Obviously, if C and P are a Hamiltonian circuit and a Hamiltonian path, respectively, then $\alpha(G\backslash C, x) = 1$ and $\alpha(G\backslash P, x) = 1$.

In the chemical literature, the graph polynomial $\beta(G, C, x)$ has been studied, which is defined as follows:

$$\beta(G, C, x) = \alpha(G, x) \mp 2\alpha(G\backslash C, x), \tag{1}$$

where C is a circuit of G. The sign "$-$" is used in the case of a so-called Hückel-type circuit, whereas the sign "$+$" is used for a so-called Möbius-type circuit. See [4] for details.

For the use of β-polynomials in chemical molecules, it is essential that all roots of these polynomials are real. In [5], Aihara mentioned that all roots of the β-polynomials are real, but gave no arguments to support his claim. In 1990, the following conjecture was proposed by Gutman and Mizoguchi in [6], and later in [7,8].

Conjecture. For any circuit C contained in any graph G, all roots of the β-polynomial of G are real.

Since then, many classes of graphs such that all roots of the β-polynomials are real have been found in [4,6–13], such as monocyclic graphs, bicyclic graphs, graphs such that no two circuits share a common edge, graphs without 3-matchings, etc., supporting the conjecture in some sense. Yet, there has been no complete solution to this conjecture. In this paper, we show that the conjecture is true in general, and therefore completely solve the conjecture.

2. Some definitions and lemmas

Definition 1 [2,3]. Let G be a graph with a vertex u. The *path tree* $T(G, u)$ is defined as follows: $T(G, u)$ is the tree with the paths in G starting at u representing the vertices, and where two such paths are joined by an edge if one is contained in the other maximally. $T(G, u)$ is called a *path tree of G with respect to u* or a *path tree of G starting at u*. Note that if G is not connected, then $T(G, u)$ is determined only by the connected component of G which contains the vertex u.

In order to give some feeling about the construction of a path tree, we would like to give the following example.

Example 1. Let G be a graph with $V(G) = \{1, 2, 3, 4, 5, 6\}$ and $E(G) = \{12, 14, 13, 24, 34, 45, 56\}$. By $T = T(G, 1)$ we denote the path tree of G starting at 1. The vertex set of T is $\{1, 12, 124, 1245, 12456, 1243, 14, 142, 143, 145, 1456, 13, 134, 1342, 1345, 13456\}$, a vertex $i_1i_2 \ldots i_k$ is adjacent to a vertex $j_1j_2 \ldots j_t$ if and only if $i_1i_2 \ldots i_k = j_1j_2 \ldots j_{t-1}$ or $i_1i_2 \ldots i_{k-1} = j_1j_2 \ldots j_t$.

In [2], the path tree $T(G, u)$ is also called a *Godsil tree*. There the following properties of $T(G, u)$ were given:

(i) $T(G, u)$ is a tree;

(ii) if G is a tree, then G and $T(G, u)$ are isomorphic; and

(iii) if $N_G(u) = \{v_1, v_2, \dots, v_r\}$ is the set of vertices adjacent to u in G, then $T(G, u)$ is isomorphic to the graph $T(G; u, N_G(u))$ obtained from the graphs $T(G \backslash u, v_i)$ $(i = 1, 2, \dots, r)$ by adjoining a new vertex u that is adjacent to each vertex corresponding to the single element path (v_i) in the graphs $T(G \backslash u, v_i)$ $(i = 1, 2, \dots, r)$.

From the above properties, we can obtain:

Lemma 1. Let G be a graph with a vertex u, and let $v_1 \in N_G(u)$. Denote by G' the graph obtained from the graphs $G - uv_1$ and $T(G \backslash u, v_1)$ by adding a new edge between the vertex u of $G - uv_1$ and the vertex (v_1) of $T(G \backslash u, v_1)$. Then $T(G, u)$ is isomorphic to $T(G', u)$.

Proof. Let $N_G(u) = \{v_1, v_2, \dots, v_r\}$. From (ii) and (iii) of the above properties, it is not difficult to see that both $T(G, u)$ and $T(G', u)$ are isomorphic to the tree $T(G; u, N_G(u))$. The details are omitted. □

Lemma 2 [3]. Let G be a graph with a vertex u. Let P be a path starting at the vertex u in the graph G and let $T = T(G, u)$. Denote by P' the unique path in T from u to P. Then

$$\frac{\alpha(G \backslash P, x)}{\alpha(G, x)} = \frac{\alpha(T \backslash P', x)}{\alpha(T, x)}.$$

The following result is well known in this subject, which will be used in our inductive proof in the next section.

Lemma 3 [6]. Let G be a monocyclic graph, and C the unique circuit of G. Then all roots of the polynomial $\beta(G, C, x)$ are real.

Remark. Note that the coefficient "2" in the β-polynomial can not be improved by a bigger constant c. For example, let G be the circuit C_4 on 4 vertices, then $\beta(G, C, x) = (x^4 - 4x^2 + 2) + c$. The discriminant is $\Delta = 4^2 - 4(2 + c) = 8 - 4c$, and hence all roots of $\beta(G, C, x)$ are real if and only if $\Delta \geqslant 0$, which implies that $c \leqslant 2$. One can find more such examples to show that the coefficient "2" is in some sense a best possible constant.

3. Main results

Theorem. For any circuit C contained in any graph G, all roots of the polynomial $\beta(G, C, x)$ are real.

Proof. For a graph G we denote by $\mathcal{C}(G)$ the set of all circuits in G and by $|\mathcal{C}(G)|$ the number of all different circuits in G. By two different circuits, we mean that one of the two circuits has at least one different edge from the other circuit. We prove this theorem by induction on the number $|\mathcal{C}(G)|$.

From lemma 3, we know that if $|\mathcal{C}(G)| = k = 1$, the theorem holds.

Suppose that the theorem holds for all graph G' such that $|\mathcal{C}(G')| \leqslant k-1$. Now, for a graph G such that $|\mathcal{C}(G)| = k \geqslant 2$, take a circuit $C \in \mathcal{C}(G)$ and let $C = v_1v_2 \ldots v_r$. Denote by P the path $v_1v_2 \ldots v_r$ in G. Note that the starting vertex v_1 could be taken as any vertex on the circuit C. We distinguish the following two cases.

Case 1. C shares a common vertex with another circuit C' of G.

Then there is a vertex v_1 on both C and C' such that an edge v_1u_1 is in C' but not in C. Denote by G' the graph obtained from the graphs $G - v_1u_1$ and $T(G\backslash v_1, u_1)$ by adding a new edge between the vertex v_1 of $G - v_1u_1$ and the vertex (u_1) of $T(G\backslash v_1, u_1)$. From lemma 1, we see that $T(G, v_1) \cong T(G', v_1)$ and C is a circuit of both G and G'. Note that $P = v_1v_2 \ldots v_r$ is a path of both G and G'. We denote by P' (respectively P'') the unique path in $T(G, v_1)$ (respectively $T(G', v_1)$) from (v_1) to P. Clearly, $P' \cong P''$ under the same isomorphism of $T(G, v_1) \cong T(G', v_1)$. Hence, from lemma 2 we have that

$$\frac{\alpha(G\backslash C, x)}{\alpha(G, x)} = \frac{\alpha(G\backslash P, x)}{\alpha(G, x)} = \frac{\alpha(T(G, v_1)\backslash P', x)}{\alpha(T(G, v_1), x)}$$

and

$$\frac{\alpha(G'\backslash C, x)}{\alpha(G', x)} = \frac{\alpha(G'\backslash P, x)}{\alpha(G', x)} = \frac{\alpha(T(G', v_1)\backslash P', x)}{\alpha(T(G', v_1), x)}.$$

Therefore,

$$\frac{\alpha(G\backslash C, x)}{\alpha(G, x)} = \frac{\alpha(G'\backslash C, x)}{\alpha(G', x)}.$$

So, we obtain that

$$\frac{\alpha(G, x) \mp 2\alpha(G\backslash C, x)}{\alpha(G, x)} = \frac{\alpha(G', x) \mp 2\alpha(G'\backslash C, x)}{\alpha(G', x)},$$

i.e.,

$$\frac{\beta(G, C, x)}{\alpha(G, x)} = \frac{\beta(G', C, x)}{\alpha(G', x)}.$$

In a clearer formula,

$$\beta(G, C, x) = \frac{\beta(G', C, x)\alpha(G, x)}{\alpha(G', x)}. \tag{2}$$

Since G' has at most $k-1$ circuits, from the induction hypothesis we know that all roots of the polynomial $\beta(G', C, x)$ are real. Also, from [2,3] we know that all roots of the polynomial $\alpha(G, x)$ are real. Hence, from formula (2) we see that all roots of the polynomial $\beta(G, C, x)$ are real.

Case 2. C does not share any common vertex with any other circuit of G.

Since G contains at least two circuits, we know that there exists at least one vertex v_1 on C such that there is a cut-edge v_1u_1 of G with the property that in $G - v_1u_1$ the connected component containing the vertex u_1 has at least one circuit C'. Denote by G' the graph obtained from the graphs $G - v_1u_1$ and $T(G\backslash v_1, u_1)$ as constructed in case 1. From lemma 1, we see that $T(G, v_1) \cong T(G', v_1)$ and C is a circuit of both G and G'. Note that $P = v_1v_2 \ldots v_r$ is a path of both G and G'. Similarly, we denote by P' (respectively P'') the unique path in $T(G, v_1)$ (respectively $T(G', v_1)$) from (v_1) to P. Clearly, $P' \cong P''$ under the same isomorphism of $T(G, v_1) \cong T(G', v_1)$. From the construction of the part $T(G\backslash v_1, u_1)$ of G', we see that the graph G' has fewer circuits than G. The rest of the proof is the same as in case 1. The proof is now complete. $\square$

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