Derivatives and Real Roots of Graph Polynomials

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Abstract

Graph polynomials are polynomials assigned to graphs. Interestingly, they also arise in many areas outside graph theory as well. Many properties of graph polynomials have been widely studied. In this paper, we survey some results on the derivative and real roots of graph polynomials, which have applications in chemistry, control theory and computer science. Related to the derivatives of graph polynomials, polynomial reconstruction of the matching polynomial is also introduced.

Keywords: graph polynomial; derivatives; real roots; polynomial reconstruction

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1 Introduction

Many kinds of graph polynomials have been introduced and extensively studied, such as characteristic polynomial, chromatic polynomial, Tutte polynomial, matching polynomial, independence polynomial, clique polynomial, etc.

Let $G$ be a simple graph with $n$ vertices and $m$ edges, whose vertex set and edge set are $V(G)$ and $E(G)$, respectively. The complement $\overline{G}$ of $G$ is the simple graph whose vertex set is $V(G)$ and whose edges are the pairs of nonadjacent vertices of $G$. For terminology and notation not defined here, we refer to [3].

Denote by $A(G)$ the adjacency matrix of $G$. The characteristic polynomial of $G$ is defined as

$$\phi(G, x) = \det(\lambda I - A(G)) = \sum_{i=0}^{n} a_i x^{n-i}.$$ 

The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\phi(G, x) = 0$ are called the eigenvalues of $G$. For more results on $\phi(G, x)$, we refer to [10, 11].
Denote by \( m(G, k) \) the \( k \)-th matching number of \( G \) for \( k \geq 0 \). We assume that \( m(G, 0) = 1 \). For \( k \geq 1 \), \( m(G, k) \) is defined as the number of ways in which \( k \) pairwise independent edges can be selected in \( G \). The matching polynomial is defined as

\[
\alpha(G, x) = \sum_{k \geq 0} (-1)^k m(G, k) x^{n-2k}.
\]

There is also an auxiliary polynomial \( \alpha(G, x, y) \), which is defined as

\[
\alpha(G, x, y) = \sum_{k \geq 0} (-1)^k m(G, k) x^{n-2k} y^k.
\]

Note that \( \alpha(G, x, y) = y^{n/2} \alpha(G, xy^{-1/2}) \). In view of this fact, we may define an auxiliary polynomial of \( \phi(G, x, y) \):

\[
\phi(G, x, y) = y^{n/2} \phi(G, xy^{-1/2}) = \sum_{k \geq 0} a_k x^{n-k} y^{k/2}.
\]

Note that \( \phi(G, x, y) \) is a polynomial in \( y \) if and only if \( G \) is bipartite.

Denote by \( n(G, k) \) the \( k \)-th independence number of \( G \) for \( k \geq 0 \). We assume that \( n(G, 0) = 1 \). For \( k \geq 1 \), \( n(G, k) \) is defined as the number of ways in which \( k \) pairwise independent vertices can be selected in \( G \). The independence polynomial is defined as

\[
\omega(G, x) = \sum_{k \geq 0} (-1)^k n(G, k) x^{n-k},
\]

which is also called independent set polynomial in \([35]\) and stable set polynomial in \([58]\). For more results on the independence polynomials, we refer the surveys \([42, 61]\).

Denote by \( c(G, k) \) the \( k \)-th clique number of \( G \) for \( k \geq 0 \). We assume that \( c(G, 0) = 1 \). For \( k \geq 1 \), \( c(G, k) \) is defined as the number of ways in which \( k \) pairwise adjacent vertices can be selected in \( G \). Note that \( c(G, 1) = n \) and \( c(G, 2) = m \). The clique polynomial is defined as

\[
c(G, x) = \sum_{k \geq 0} (-1)^k c(G, k) x^{n-k}.
\]

Note that the clique polynomial of a graph \( G \) is exactly the independence polynomial of the complement \( \overline{G} \) of \( G \), i.e., \( c(G, x) = \alpha(\overline{G}, x) \). Obviously, we also have

\[
c(G, x) + c(\overline{G}, x) = \alpha(G, x) + \alpha(\overline{G}, x).
\]

The following results are easily obtained.

**Theorem 1.** Let \( G_1 \) and \( G_1 \) be two vertex-disjoint graphs. Then we have

\[
c(G_1 \cup G_2, x) = c(G_1, x) + c(G_2, x) - 1, \quad \alpha(G_1 \cup G_2, x) = \alpha(G_1, x) \cdot \alpha(G_2, x);
\]

\[
c(G_1 + G_2, x) = c(G_1, x) \cdot c(G_2, x), \quad \alpha(G_1 + G_2, x) = \alpha(G_1, x) + \alpha(G_2, x) - 1.
\]
In [35], the authors obtained the following similar result.

**Theorem 2.** Let $G_1$ and $G_2$ be two vertex-disjoint graphs with $n_1$ and $n_2$ vertices, respectively. Then

$$c(G_1 \times G_2, x) = n_2 \cdot c(G_1, x) + n_1 \cdot c(G_2, x) - (n_1 + n_2 + n_1n_2x) + 1.$$  

For more properties on $c(G, x)$ and $\alpha(G, x)$, we refer to [35].

Many properties of graph polynomials have been widely studied. In this paper, we survey some results on the derivative and real roots of graph polynomials, which have applications in chemistry, control theory and computer science. Related to the derivatives of graph polynomials, polynomial reconstruction of the matching polynomial is also introduced.

## 2 Derivatives of graph polynomials

The derivatives of the characteristic polynomial were examined by Clarke [9] and the following result was showed.

**Theorem 3.** Let $G$ be a simple graphs and $\phi(G, x)$ be the characteristic polynomial of $G$. Then

$$\frac{d\phi(G, x)}{dx} = \sum_{v \in V(G)} \phi(G - v, x).$$

Gutman and Hosoya [28] got a similar result for the matching polynomial.

**Theorem 4.** Let $G$ be a simple graphs and $\alpha(G, x)$ be the matching polynomial of $G$. Then

$$\frac{d\alpha(G, x)}{dx} = \sum_{v \in V(G)} \alpha(G - v, x).$$

One can get the first derivative of the independence polynomial and clique polynomial, which have similar expressions as the matching polynomial and characteristic polynomial. That is,

$$\frac{d\omega(G, x)}{dx} = \sum_{v \in V(G)} \omega(G - v, x), \quad \frac{dc(G, x)}{dx} = \sum_{v \in V(G)} c(G - v, x).$$

Although the four first derivatives obey fully analogous expressions, their proofs existing in the literatures, are quite dissimilar. Li and Gutman [44] provided a unified approach to all these formulas by introducing a general graph polynomial.

Let $f$ be a complex-valued function defined on the set of graphs $\mathcal{G}$ such that $G_1 \cong G_2$ implies $f(G_1) = f(G_2)$. Let $G$ be a graph on $n$ vertices and $S(G)$ be the set of all subgraphs of $G$. Define

$$S_k(G) = \{H : H \in S(G) \text{ and } |V(H)| = k\}, \quad p(G, k) = \sum_{H \in S_k(G)} f(H).$$
Then, the general graph polynomial of $G$ is defined as

$$P(G, x) = \sum_{k=0}^{n} p(G, k)x^{n-k}.$$ 

Actually, let

$$f(H) = \begin{cases} (-1)^{|V(H)|/2} & \text{if } H \text{ is 1-regular;} \\ 0 & \text{otherwise.} \end{cases}$$

Then the resulting polynomial is the matching polynomial. Let

$$f(H) = \begin{cases} (-1)^{|V(H)|} & \text{if } H \text{ is no edges;} \\ 0 & \text{otherwise.} \end{cases}$$

Then the resulting polynomial is the independence polynomial. Let

$$f(H) = \begin{cases} (-1)^{r(H)} \cdot 2^{c(H)} & \text{if all components of } H \text{ are 1- or 2-regular;} \\ 0 & \text{otherwise,} \end{cases}$$

where $r(H)$ is the number of components in $H$ and $c(H)$ is the number of cycles in $H$. Then the resulting polynomial is the characteristic polynomial. Let

$$f(H) = \begin{cases} (-1)^{|V(H)|} & \text{if } H \text{ is a complete graph;} \\ 0 & \text{otherwise.} \end{cases}$$

Then the resulting polynomial is the clique polynomial.

The following theorem was obtained by Li and Gutman in [44].

**Theorem 5.** For the graph polynomial $P(G, x)$ of $G$, we have

$$\frac{d}{dx} (P(G, x)) = \sum_{v \in V(G)} P(G - v, x).$$

Furthermore, Gutman [24, 27] got the first derivative formula for $\alpha(G, x, y)$:

$$\partial \alpha(G, x, y) / \partial y = - \sum_{uv \in E(G)} \alpha(G - u - v, x, y).$$

To find an expression for $\partial \phi(G, x, y) / \partial y$ of a bipartite graph was posed by Gutman as a problem in [23]. A solution of this problem was offered by Li and Zhang [48].

**Theorem 6.** For a bipartite graph $G$,

$$\partial \phi(G, x, y) / \partial y = - \sum_{uv \in E(G)} \phi(G - u - v, x, y) - \sum_{C \subseteq G} n(C) y^{n(C)/2-1} \phi(G - C, x, y),$$

where $C$ is a cycle, possessing $n(C)$ vertices.
The above theorem was proved by using Sachs Theorem for the coefficients of the characteristic polynomial and by verifying the equality of the respective coefficients of the polynomials on the left- and right-hand sides of Eq. (1). In [29], the authors put forward another route to Eq. (1), from which it become evident that Eq. (1) holds for an arbitrary graph.

Moreover, if we define
\[ P(G, x, y) = \sum_{i+j=n} p(G, k)x^iy^j, \]
then we can obtain
\[ \frac{\partial P(G, x, y)}{\partial y} = ny^{-1}P(G, x, y) - xy^{-1} \sum_{v \in V(G)} P(G - v, x, y). \]

Derivatives of other graph polynomials have also been studied, such as the cube polynomial [5], the Tutte polynomial [15], the Wiener polynomial [39], etc.

3 Polynomial reconstruction of the matching polynomial

The derivative of a graph polynomial is related the problem of polynomial reconstruction. This section aims to prove that graphs with pendant edges are polynomial reconstructible and, on the other hand, to display some evidence that arbitrary graphs are not, which is given in [47].

The famous (and still unsolved) reconstruction conjecture of Kelly [38] and Ulam [63] states that every graph \( G \) with at least three vertices can be reconstructed from (the isomorphism classes of) its vertex-deleted subgraphs.

With respect to a graph polynomial \( P(G) \), this question may be adapted as follows: Can \( P(G) \) of a graph \( G = (V, E) \) be reconstructed from the graph polynomials of the vertex deleted-subgraphs, that is from the collection \( P(G-v) \) for \( v \in V \)? Here, this problem is considered for the matching polynomial of a graph. For results about the polynomial reconstruction of other graph polynomials, see the article by Brešar, Imrich, and Klavžar [4, Section 1] and the references therein. For additional results, see [59, Section 7] [60, Subsection 4.7.3].

The matching polynomial we considered here is the generating function of the number of its matchings with respect to their cardinality, denoted by \( M(G, x, y) \), which is different from the above \( \alpha(G, x) \) and \( \alpha(G, x, y) \). Let \( G = (V, E) \) be a graph. A matching in \( G \) is an edge subset \( A \subseteq E \), such that no two edges in \( A \) have a common vertex. The matching polynomial \( M(G, x, y) \) is defined as
\[ M(G, x, y) = \sum_{A \subseteq E \text{ is a matching}} x^{\text{def}(G, A)}y^{|A|}, \]
where \( \text{def}(G, A) = |V| - |\bigcup_{e \in A} e| \) is the number of vertices not included in any of the edges of \( A \). A matching \( A \) is a perfect matching, if its edges include all vertices, that means if \( \text{def}(G, A) = 0 \). A near-perfect matching \( A \) is a matching that includes all vertices except one, that means \( \text{def}(G, A) = 1 \). For more information about matchings and the matching polynomial, see [17, 22, 51].

For a graph \( G = (V, E) \) with a vertex \( v \in V \), \( G_{-v} \) is the graph arising from the deletion of \( v \), i.e., arising by the removal of \( v \) and all the edges incident with \( v \). The multiset of (the isomorphism classes of) the vertex-deleted subgraphs \( G_{-v} \) for \( v \in V \) is the deck of \( G \). The polynomial deck \( D_P(G) \) with respect to a graph polynomial \( P(G) \) is the multiset of \( P(G_{-v}) \) for \( v \in V \). A graph polynomial \( P(G) \) is polynomial reconstructible, if \( P(G) \) can be determined from \( D_P(G) \).

By arguments analogous to those used in Kelly’s Lemma [38], the derivative of the matching polynomial of a graph \( G = (V, E) \) equals the sum of the polynomials in the corresponding polynomial deck.

**Proposition 1** (Lemma 1 in [18]). Let \( G = (V, E) \) be a graph. The matching polynomial \( M(G, x, y) \) satisfies

\[
\frac{\delta}{\delta x} M(G, x, y) = \sum_{v \in V} M(G_{-v}, x, y).
\]

In other words, all coefficients of the matching polynomial except the one corresponding to the number of perfect matchings can be determined from the polynomial deck and thus also from the deck:

\[
m_{i,j}(G) = \frac{1}{i} \sum_{v \in V} m_{i,j}(G_{-v}) \quad \forall i \geq 1,
\]

where \( m_{i,j}(G) \) is the coefficient of the monomial \( x^i y^j \) in \( M(G, x, y) \).

Consequently, the (polynomial) reconstruction of the matching polynomial reduces to the determination of the number of perfect matchings.

**Proposition 2.** The matching polynomial \( M(G, x, y) \) of a graph \( G \) can be determined from its polynomial deck \( D_M(G) \) and its number of perfect matchings. In particular, the matching polynomial \( M(G, x, y) \) of a graph with an odd number of vertices is polynomial reconstructible.

Tutte [62, Statement 6.9] showed that the number of perfect matchings of a simple graph can be determined from its deck of vertex-deleted subgraphs and therefore gave an affirmative answer on the reconstruction problem for the matching polynomial.

The matching polynomial of a simple graph can also be reconstructed from the deck of edge-extracted and edge-deleted subgraphs [18, Theorem 4 and 6] and from the polynomial
deck of the edge-extracted graphs [24, Corollary 2.3]. For a simple graph $G$ on $n$ vertices, the matching polynomial is reconstructible from the collection of induced subgraphs of $G$ with $\lfloor \frac{n}{2} \rfloor + 1$ vertices [20, Theorem 4.1].

The following result is from [47] for simple graphs with pendant edges.

**Theorem 7.** Let $G = (V, E)$ be a simple graph with a vertex of degree 1. Then, $G$ has a perfect matching if and only if each vertex-deleted subgraph $G_{-v}$ for $v \in V$ has a near-perfect matching.

As proved recently by Huang and Lih [36], this statement can be generalized to arbitrary simple graphs.

**Corollary 8.** Let $G = (V, E)$ be a forest. Then $G$ has a perfect matching if and only if each vertex-deleted subgraph $G_{-v}$ for $v \in V$ has a near-perfect matching.

Forests have either none or one perfect matching, because every pendant edge must be in a perfect matching (in order to cover the vertices of degree 1) and the same holds recursively for the subforest arising by deleting all the vertices of the pendant edges. Therefore, from Proposition 2 and Corollary 8, the polynomial reconstructibility of the matching polynomial follows.

**Corollary 9.** The matching polynomial $M(G, x, y)$ of a forest is polynomial reconstructible.

On the other hand, arbitrary graphs with pendant edges can have more than one perfect matching. However, Corollary 8 can be extended to obtain the number of perfect matchings. For a graph $G = (V, E)$, the number of perfect matchings and of near-perfect matchings of $G$ is denoted by $p(G)$ and $np(G)$, respectively.

**Theorem 10.** Let $G = (V, E)$ be a simple graph with a pendant edge $e = \{u, w\}$ where $w$ is a vertex of degree 1. Then we have

$$p(G) = np(G_{-u}) \leq np(G_{-v}) \quad \forall v \in V$$

and particularly

$$p(G) = \min \{np(G_{-v}) \mid v \in V\}.$$  

By applying this theorem, the number of perfect matchings of a simple graph with pendant edges can be determined from its polynomial deck and the following result is obtained as a corollary.

**Corollary 11.** The matching polynomial $M(G, x, y)$ of a simple graph with a pendant edge is polynomial reconstructible.
While it is true that the matching polynomials of graphs with an odd number of vertices or with a pendant edge are polynomial reconstructible, it does not hold for arbitrary graphs.

There are graphs which have the same polynomial deck and yet their matching polynomials are different. Although there are already counterexamples with as little as six vertices, it seems that nothing has been published before in connection with the question addressed here.

**Remark 1.** The matching polynomial $M(G, x, y)$ of an arbitrary graph is not polynomial reconstructible. The minimal counterexample for simple graphs (with respect to the number of vertices and edges) are constructed in \[47\].

The question arises here: whether or not there are such counterexamples consisting of graphs with an arbitrary even number of vertices. In \[47\], we gave an affirmative answer to this question.

## 4 Roots of beta-polynomials and independence polynomials

Polynomials whose all zeros are real-valued numbers are said to be real. Several graph polynomials have been known to be real; among them the matching polynomial $\alpha(G, x)$ plays a distinguished role \[21, 34\].

Polynomials with only real roots arise in various applications in control theory and computer science \[65\], but also admit interesting mathematical properties on their own. Newton noted that the sequence of coefficients of such polynomials form a log-concave (and hence unimodal) sequence. These polynomials also have strong connections to totally positive matrices.

The fact that for all graphs, all zeros of the matching polynomial are real-valued was first established by Heilmann and Lieb \[34\].

Let $C$ be a circuit contained in a graph $G$. If $C$ is a Hamiltonian cycle, then $\alpha(G - C, x) \equiv 1$. In certain considerations in theoretical chemistry \[1, 40, 54, 55\], graph polynomials $\beta(G, C, x)$ are encountered, defined as

$$\beta(G, C, x) = \alpha(G, x) - 2\alpha(G - C, x) \tag{6}$$

and

$$\beta(G, C, x) = \alpha(G, x) + 2\alpha(G - C, x) \tag{7}$$

Formula (6) is used in the case of so-called Hückel-type circuits, whereas formula (7) for the so-called Möbius-type circuits. For details, see \[54\]. These polynomials are also called **circuit characteristic polynomials** \[1\].
Already in the first paper devoted to this topic [11], Aihara mentioned that the zeros of the \( \beta \)-polynomials are real-valued, but gave no argument to support his claim. In the meantime, for a number of classes of graphs it was shown that \( \beta(G, C, x) \) is indeed a real polynomial [25, 26, 30, 40, 49, 55, 41]. In addition to this, by means of extensive computer searches not a single graph with non-real \( \beta \)-polynomial could be detected. The following conjecture has been put forward by Gutman and Mizoguchi in [25, 26, 30].

**Conjecture 1.** For any circuit \( C \) contained in any graph \( G \), the \( \beta \)-polynomials \( \beta(G, C, x) \), Eqs. (6) and (7), are real.

Many results have been obtained. In particular, \( \beta(G, C, x) \) has been shown to be real for unicyclic graphs [30], bicyclic graphs [55], graphs in which no edge belongs to more than one circuit [55], graphs without 3-matchings (i.e., \( m(G, 3) = 0 \)) [40], several (but not all) classes of graphs without 4-matchings (i.e., \( m(G, 4) = 0 \)) [41].

In [46], Li et al. showed that the conjecture is true for complete graphs. Actually, they proved a stronger result for complete graphs.

**Theorem 12.** For any circuit \( C \) in the complete graph \( K_n \), the polynomial

\[
\beta(K_n, C, t; x) = \alpha(K_n, x) + t\alpha(K_n - C, x)
\]

is real for any real \( t \) such that \(|t| \leq n - 1\).

The proof offered in [46] relies on an earlier published theorem by Turán. In [45], Li and Gutman presented an elementary self-contained proof for complete graphs. Finally, in [50], Li et al. showed that the conjecture is true for all graphs, and therefore completely solved this conjecture.

**Theorem 13.** For any circuit \( C \) contained in any graph \( G \), all roots of the polynomial \( \beta(G, C, x) \) are real.

Chudnovsky and Seymour [8] proved the following result for independence polynomial.

**Theorem 14.** If \( G \) is clawfree, then all roots of its independence polynomial are real.

Theorem 14 extends a theorem of [34], answering a question posed by Hamidoune [33] and Stanley [58]. Since all line graphs are clawfree, this extends the result of [34]. Later, Levit and Mandrescu studied the roots of independence polynomials of almost all very well-covered graphs [43]. In [53], Mandrescu showed that starting from a graph \( G \) whose independence polynomial has only real roots, one can build an infinite family of graphs, whose independence polynomials have only real roots.

Real roots of other graph polynomials have also been extensively studied, such as edge-cover polynomial [2], the expected independence polynomial [7], domination polynomial...
sigma-polynomial [67], chromatic polynomial [14] [37] [66], Wiener polynomial [12], flow polynomial [37], Tutte polynomial [16] [64], etc. For more results on the roots of graph polynomials, we refer to [13] [31] [32] [52] [56] [57] [65].

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