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THE β-POLYNOMIALS OF COMPLETE GRAPHS ARE REAL

Xueliang Li, Ivan Gutman and Gradimir V. Milovanović

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ABSTRACT. A polynomial is said to be real if all its zeros are real. It has been conjectured that the β-polynomials of all graphs are real. In this paper we show that the conjecture is true for complete graphs. In fact, we obtain a more general result, namely that certain linear combinations of Hermite polynomials are real.

Introduction

Polynomials whose all zeros are real-valued numbers are said to be real. Several graphic polynomials are known to be real; among them the matching polynomial plays a distinguished role [3,4,9].

Let G be a graph on n vertices. The *matching polynomial* of G is defined as [3]:

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

where $m(G,k)$ is the number of k-matchings of G, i.e., the number of ways in which k mutually non-touching edges are selected in G; $m(G,0) = 1$ and $m(G,1) =$ number of edges of G.

The fact that for all graphs, all zeros of the matching polynomial are real-valued has been first established by Heilmann and Lieb [9]; see also [3,4].

Let C be a circuit contained in the graph G. The subgraph obtained by deleting the vertices of C from G is denoted by $G \smallsetminus C$. The number of vertices of C will be denoted by m. Then $G \smallsetminus C$ possesses $n - m$ vertices.

If C is a Hamiltonian circuit, i.e., if $m = n$ then, by definition, $\alpha(G \smallsetminus C, x) \equiv 1$.

In certain considerations in theoretical chemistry [2,11,14,15], graphic polynomials $\beta(G,C,x)$ are encountered, defined as

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

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and

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

These have been named [2] *circuit characteristic polynomials*, but in this work we call them simply *β-polynomials*. Formula (1) is used in the case of so-called Hückel-type circuits whereas formula (2) for so-called Möbius-type circuits; for more details see [14].

For the success of the chemical theory in which β-polynomials occur, it is essential that these polynomials are real. Already in the first paper devoted to this topic [2], Aihara mentioned that the zeros of the β-polynomials were 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 [5,6,8,11,12,13,15]. In addition to this, by means of extensive computer searches not a single graph with non-real β-polynomial could be detected. The following conjecture has been put forward [5,6,8]:

CONJECTURE. *For any circuit C contained in any graph G, the β-polynomials $\beta(G,C,x)$, equations* (1) *and* (2), *are real.*

Up to the present moment this conjecture has neither been proved nor disproved (although a prize is offered for its solution [8]). On the other hand, many results, corroborating its validity, have been obtained. Thus, in particular, $\beta(G,C,x)$ has been shown to be real for:

- unicyclic graphs [8];
- bicyclic graphs [15];
- graphs in which no edge belongs to more than one circuit [15];
- graphs without 3-matchings ($m(G,3)=0$) [11];
- several (but not all) classes of graphs without 4-matchings ($m(G,4)=0$) [12].

Note that the aforementioned graphs have comparatively few edges. A natural question is whether or not the conjecture is true for dense graphs. The extreme case in this direction is the complete graph. In this work we show that the conjecture is obeyed by complete graphs.

The main result

THEOREM 1. *Let K_n be the complete graph on n vertices and C any of its circuits. Then $\beta(K_n,C,x)$, equations* (1), (2), *is a real polynomial.*

Instead of Theorem 1 we demonstrate the validity of a stronger result, namely Theorem 2. In order to state it we need some preparations.

If C is a circuit on m vertices, then $K_n\smallsetminus C=K_{n-m}$, implying that

$$\beta(K_n,C,x)=\alpha(K_n,x)\pm 2\,\alpha(K_{n-m},x) \tag{3}$$

Now, a well-known result from the theory of matching polynomial is [4,7,9,10]:

$$\alpha(K_n,x)=He_n(x) \tag{4}$$

where He_n is one of the standard forms of the Hermite polynomial [1, p. 778]. Such (monic) Hermite polynomials are orthogonal on $(-\infty, +\infty)$ with respect to the weight function $e^{-x^2/2}$.

Bearing in mind equations (4) and (4) we define a polynomial

$$\beta(n, m, t, x) = He_n(x) + t\, He_{n-m}(x), \tag{5}$$

where $1 \leq m \leq n$ and t is a real number. Clearly, for $n \geq 3$, $|t| = 2$ and $3 \leq m \leq n$, equation (5) is the β-polynomial of the complete graph on n vertices, pertaining to a circuit with m vertices.

THEOREM 2. *For all (positive integer) values of n, for all $m = 1, 2, \ldots, n$ and for $|t| \leq n - 1$ the polynomial $\beta(n, m, t, x)$, equation (5), is real.*

Obviously, Theorem 1 is a special case of Theorem 2. Therefore in what follows we proceed towards proving Theorem 2. It should be noted that the right-hand side of equation (5) is a sort of linear combination of Hermite polynomials.

Preparations

Some well known properties [1] of the Hermite polynomials are summarized in Lemma 1.

LEMMA 1. *(i) The Hermite polynomials $He_n(x)$ satisfy the three-term recurrence relation*

$$He_n(x) = x\, He_{n-1}(x) - (n-1)\, He_{n-2}(x);$$

(ii) All zeros of $He_n(x)$ are real and distinct;
(iii)

$$\frac{d}{dx} He_n(x) = n\, He_{n-1}(x)$$

and hence, $He_n(x)$ has a local extreme x_i if and only if $He_{n-1}(x_i) = 0$. So, the extremes of $He_n(x)$ are distinct.

Throughout this paper $x_1, x_2, \ldots, x_{n-1}$ denote the distinct zeros of $He_{n-1}(x)$.
From equation (4) and Theorem 7 of [4], we have

LEMMA 2. *$|x_i| < 2\sqrt{n-3}$ holds for all $i = 1, 2, \ldots, n-1$ and $n \geq 4$.*

LEMMA 3. *If for all $i = 1, 2, \ldots, n-1$, the sign of*

$$\beta(n, m, t, x_i) = He_n(x_i) + t\, He_{n-m}(x_i)$$

is the same as that of $He_n(x_i)$, then $\beta(n, m, t, x)$ is real.

Proof. From Lemma 1 (iii), we have that x_i, $i = 1, 2, \ldots, n-1$ are the extremes of $He_n(x)$. Since $He_n(x)$ does not have multiple zeros (Lemma 1 (ii)), we know that $He_n(x_i) \neq 0$ for all $i = 1, 2, \ldots, n-1$, and that $He_n(x_i)$ and $He_n(x_{i+1})$ have different signs, $i = 1, 2, \ldots, n-2$.

From the definition of $\beta(n, m, t, x)$ and the condition of Lemma 3, we deduce that $\beta(n, m, t, x)$ has at least as many real zeros as $He_n(x)$, that is at least n real zeros. On the other hand the degree of $\beta(n, m, t, x)$ is n. $\square$

LEMMA 4. *If $|He_n(x_i)| > (n-1)\,|He_{n-m}(x_i)|$ for all $i = 1,2,\ldots,n-1$, then $\beta(n,m,t,x)$ is real for $|t| \le n-1$.*

Proof. Since $|He_n(x_i)| > (n-1)\,|He_{n-m}(x_i)| \ge |t|\,|He_{n-m}(x_i)|$ for all $i = 1,2,\ldots,n-1$, the sign of $\beta(n,m,t,x_i) = He_n(x_i) + t\,He_{n-m}(x_i)$ depends only on the sign of $He_n(x_i)$. Lemma 4 follows from Lemma 3. □

Proof of Theorem 2

Bearing in mind that $He_{n-1}(x_i) = 0$, from Lemma 4 we directly get

LEMMA 5. *The polynomial $\beta(n,1,t,x)$ is real for $n \ge 1$ and any real value of the parameter t.*

Lemma 5 implies the validity of Theorem 2 for $m = 1$. What remains is to consider the case $m \ge 2$. Therefore, in what follows it will be assumed that $2 \le m \le n$.

Define the auxiliary quantities $a_{n,m}$ as

$$a_{n,m} = \max_{1\le i\le n-1} \left| \frac{He_{n-m}(x_i)}{He_n(x_i)} \right| \tag{6}$$

Because of Lemma 5, if

$$a_{n,m} \le \frac{1}{n-1} \tag{7}$$

then $\beta(n,m,t,x)$ is real for $|t| \le n-1$. Therefore, in order to complete the proof of Theorem 2 we only need to verify the inequality (7).

Using the well-known three-term recurrence relation for the Hermite polynomials (Lemma 1), equation (6) reduces to

$$a_{n,m} = \frac{1}{n-1} \max_{1\le i\le n-1} \left| \frac{He_{n-m}(x_i)}{He_{n-2}(x_i)} \right| = \frac{1}{(n-1)(n-2)} \max_{1\le i\le n-1} \left| \frac{x_i\, He_{n-m}(x_i)}{He_{n-3}(x_i)} \right|$$

and we conclude immediately that

$$a_{n,1} = 0\ , \qquad a_{n,2} = \frac{1}{n-1} \quad (n \ge 2)\ ,$$

and

$$a_{n,3} = \frac{1}{(n-1)(n-2)} \max_{1\le i\le n-1} |x_i| \begin{cases} = \dfrac{1}{n-1}\,, & n = 3, \\[2ex] < \dfrac{2\sqrt{n-3}}{(n-1)(n-2)} \le \frac{1}{n-1}\,, & n \ge 4. \end{cases}$$

Note that the relation $a_{n,1} = 0$ provides another proof of Lemma 5. The upper bound for $a_{n,3}$ follows from Lemma 2.

The case when $n \geq m \geq 4$ can be verified using a result of Turán [17] (see also [16]). Namely, under the condition

$$\sum_{k=0}^{n-2} k!\, c_k^2 \;<\; (n-1)!\, c_n^2 \,,$$

Turán proved that the polynomial $P(z) = \sum_{k=0}^{n} c_k\, He_k(z)$ has n distinct real zeros. Considering the β-polynomial given by (5), we conclude that it has all real zeros if $|t| < \sqrt{(n-1)!/(n-m)!}$. On the other hand, it is easily verified that for $n > m \geq 4$ the expression $\sqrt{(n-1)!/(n-m)!}$ is greater than $n-1$.

Notice that $a_{4,4} = 1/3$.

By this, the proof of Theorem 2 has been completed. $\square$

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References

[1] M. Abramowitz, I. A. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1972.

[2] J. Aihara, *Resonance energies of benzenoid hydrocarbons*, J. Am. Chem. Soc. **99** (1977) 2048–2053.

[3] D. Cvetković, M. Doob, I. Gutman, A. Torgašev, *Recent Results in the Theory of Graph Spectra*, North–Holland, Amsterdam, 1988.

[4] C. D. Godsil, I. Gutman, *On the theory of the matching polynomial*, J. Graph Theory **5** (1981) 137–144.

[5] I. Gutman, *A contribution to the study of real graph polynomials*, Publ. Elektrotehn. Fak. (Beograd) Ser. Mat. **3** (1992) 35–40.

[6] I. Gutman *A real graph polynomial?*, Graph Theory Notes New York **22** (1992) 33–37.

[7] I. Gutman, D. M. Cvetković *Relations between graphs and special functions*, Coll. Sci. Papers Fac. Sci. Kragujevac **1** (1980) 101–119.

[8] I. Gutman, N. Mizoguchi, *A property of the circuit characteristic polynomial*, J. Math. Chem. **5** (1990) 81–82.

[9] O. J. Heilmann, E. H. Lieb, *Theory of monomer–dimer systems*, Commun. Math. Phys. **25** (1972) 190–232.

[10] H. Hosoya, *Graphical and combinatorial aspects of some orthogonal polynomials*, Nat. Sci. Repts. Ochanomizu Univ. **31** (1981) 127–138.

[11] M. Lepović, I. Gutman, M. Petrović, N. Mizoguchi, *Some contributions to the theory of cyclic conjugation*, J. Serb. Chem. Soc. **55** (1990) 193–198.

[12] M. Lepović, I. Gutman, M. Petrović, *A conjecture in the theory of cyclic conjugation and an example supporting its validity*, Commun. Math. Chem. (MATCH) **28** (1992) 219–234.

[13] X. Li, B. Zhao, I. Gutman, *More examples for supporting the validity of a conjecture on β-polynomial*, J. Serb. Chem. Soc. **60** (1995) 1095–1101.

[14] N. Mizoguchi, *Unified rule for stability of Hückel–type and Möbius–type systems*, J. Phys. Chem. **92** (1988) 2754–2756.

[15] N. Mizoguchi, *Circuit resonance energy. On the roots of circuit characteristic polynomial*, Bull. Chem. Soc. Japan **63** (1990) 765–769.

[16] G. Schmeisser, *Inequalities for the zeros of an orthogonal expansion of a polynomial*, in: G. V. Milovanović (Ed.), *Recent Progress in Inequalities*, Kluwer, Dordrecht, 1998, pp. 381–396.

[17] P. Turán, *To the analytic theory of algebraic equations*, Izv. Mat. Inst. Bulgar. Akad. Nauk **3** (1958) 123–137.

Xueliang Li
Department of Applied Mathematics
Northwestern Polytechnical University
X'ian, Shaanxi 710072
P.R. China
iamlxl@nwpu.edu.cn

Ivan Gutman
Prirodno-matematički fakultet
34001 Kragujevac, p.p. 60
Yugoslavia
gutman@knez.uis.kg.ac.yu

Gradimir V. Milovanović
Elektronski fakultet
18001 Niš, p.p. 73
Yugoslavia
grade@gauss.elfak.ni.ac.yu

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