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EDGE ERASURE TECHNIQUE FOR COMPUTING THE CHARACTERISTIC POLYNOMIALS OF MOLECULAR GRAPHS

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A b s t r a c t

The reconstruction of the characteristic polynomial of a graph from the characteristic polynomials of its edge deleted subgraphs is examined. Two results along these lines are given, showing that the reconstruction is possible in the case of all acyclic and all non-alternant monocyclic molecular graphs.

Introduction

Randić recently[1] proposed a new technique for the calculation of the characteristic polynomial of a graph. Let G be a graph, $v_1, v_2, \dots, v_n$ its vertices and Ch(G) = = Ch(G, x) its characteristic polynomial[2]. According to the method of Randić, in order to calculate Ch(G) one has first to determine the characteristic polynomials of $G-v_1$, $G-v_2, \dots, G-v_n$ and then to use the well-known relation[2,3,4]

$$\sum_{i=1}^{n} \mathrm{Ch}(G-v_i) = \mathrm{Ch}'(G) \qquad (1)$$

where Ch´(G) is the first derivative of Ch(G) with respect to the variable x.

The characteristic polynomial of G can be now obtained from the expression

$$\mathrm{Ch}(G, x) = \sum_{i=1}^{n} \int_0^x \mathrm{Ch}(G-v_i)\, dx + \mathrm{Ch}(G, 0) \ ,$$

provided the constant Ch(G, O) is known. The difficulty of Randić´s method lies just in the fact that Ch(G, O) needs not be known and that in the general case we are (at the present moment) not able to calculate Ch(G, O) from the polynomials $\mathrm{Ch}(G-v_i)$, $i=1,2,\dots,n$.

The question whether Ch(G) can be reconstructed from the knowledge of $Ch(G-v_i)$, $i=1,2,\ldots,n$ (and without exploiting any other information about the structure of the graph G) was first considered by Cvetković and one of the present authors[4]. Although several particular results along these lines have been obtained[4,5], a general solution is still missing.

The reconstruction of the characteristic polynomial of a molecular graph and problems related to eq. (1) have been discussed in some detail in the chemical literature[1,6,7].

A new reconstruction problem and some partial solutions

In this paper we shall be concerned with another variant of the reconstruction problem. Let the edges of the graph G be labeled by $e_1, e_2, \ldots, e_m$.

P r o b l e m. Does the collection of polynomials $Ch(G-e_1)$, $Ch(G-e_2), \ldots, Ch(G-e_m)$ determine a unique polynomial Ch(G) ? Is it possible to calculate Ch(G) from the knowledge of $Ch(G-e_j)$, $j=1,2,\ldots,m$?

For m = 2 the answer to the above questions is negative. Namely, the graphs G_1 and G_2 have identical edge-deleted subgraphs, whereas their characteristic polynomials are different: $Ch(G_1) = x^4 - 2x^2$, $Ch(G_2) = x^4 - 2x^2 + 1$.

G_1 G_2

For m > 2 we offer the following two partial answers to our questions.

Proposition 1 a. If we know that G is an acyclic graph, then Ch(G) can be reconstructed from the polynomials $Ch(G-e_j)$, $j=1,2,...,m$.

Proposition 2a. If we know that G is a monocyclic graph whose cycle has odd size, then Ch(G) can be reconstructed from the polynomials $Ch(G-e_j)$, $j=1,2,...,m$.

Before proving these propositions we shall describe the actual method by which the coefficients of Ch(G) can be calculated from the coefficients of $Ch(G-e_j)$.

Let $P(x) = a_o\, x^n + a_1\, x^{n-1} + a_2\, x^{n-2} + \cdots + a_n$ be a polynomial. Then we write: $\mathrm{coef}_k\, P(x) = a_k$.

Let $p\, G_a \dot{+} q\, G_b$ denote a graph having $p + q$ components, p of which are isomorphic to G_a and q of which are isomorphic to G_b. Let in addition P_n and C_n denote the path and the cycle, respectively, with n vertices. (For example, $G_1 = P_3 \dot{+} P_1$ and $G_2 = 2\, P_2$.)

P r o p o s i t i o n 1 b. If G is an acyclic graph with m edges, then

$$\mathrm{coef}_{2k}\ \mathrm{Ch}(G) = \frac{1}{m-k}\ \mathrm{coef}_{2k} \sum_{j=1}^{m} \mathrm{Ch}(G-e_j)$$

for $k \geq 0$, $k \neq m$, and, of course,

$$\mathrm{coef}_{2k+1}\ \mathrm{Ch}(G) = 0$$

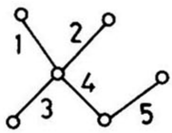
for $k \geq 0$. In addition,

$$\mathrm{coef}_{2m}\ \mathrm{Ch}(G) = 0$$

except if $G = m\ P_2 \dot{+} (n-2m)\ P_1$.

From the collection of polynomials $\mathrm{Ch}(G-e_j)$, $j=1,2,...m$ one can easily recognize whether G has the form $m\ P_2 \dot{+} (n-2m)\ P_1$ or not. In this exceptional case, $\mathrm{coef}_{2m}\ \mathrm{Ch}(G) = (-1)^m$. The only molecular graph which belongs to this exceptional class is, of course, P_2.

For example, consider the molecular graph G_3 of 2,2-dimethylbuthane, whose characteristic polynomial is $\mathrm{Ch}(G_3) = x^6 - 5\ x^4 + 3\ x^2$.



G_3

j	$G_3 - e_j$	$Ch(G_3 - e_j)$
1,2,3		$(x)(x^5 - 4x^3 + 2x)$
4		$(x^4 - 3x^2)(x^2 - 1)$
5		$(x^5 - 4x^3)(x)$

$$\sum_{j=1}^{5} Ch(G_3 - e_j) = 5x^6 - 20x^4 + 9x^2$$

$$Ch(G_3) = (5/5)x^6 - (20/4)x^4 + (9/3)x^2 - (0/2)$$

P r o p o s i t i o n 2 b. If G is a monocyclic graph whose cycle C is of size r and r is odd, then

$$\mathrm{coef}_{2k}\, Ch(G) = \frac{1}{m-k}\, \mathrm{coef}_{2k} \sum_{j=1}^{m} Ch(G - e_j) \tag{2}$$

for $k \geq 0$, $k \neq m$,

$$\mathrm{coef}_k\, Ch(G) = 0$$

for $k = 2m$ and $k = 1,3,\ldots,r-2$, and

$$\mathrm{coef}_{r+2k}\, Ch(G) = \frac{1}{m-r-k}\, \mathrm{coef}_{r+2k} \sum_{j=1}^{m} Ch(G - e_j) \tag{3}$$

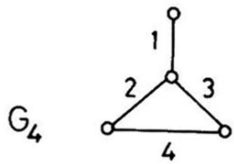
for $k \geq 0$, $k \neq m-r$. In addition,

$$\mathrm{coef}_{2m-r}\, Ch(G) = 0$$

except if G is of the form $C_r \dot{+} (m-r)\ P_2 \dot{+} (n+r-2m)\ P_1$.

From the polynomials $Ch(G-e_j)$, $j=1,2,\ldots,m$ one can easily decide whether the graph G is of the above form or not. If this is the case, then $coef_{2m-r}\ Ch(G) = -2\ (-1)^{m-r}$. The only molecular graph which belongs to this exceptional class is C_n.

From Proposition 2 we see that it is possible to reconstruct the characteristic polynomial of all graphs which represent non-alternant monocyclic molecules. For example, consider the molecular graph G_4 of methylcyclopropane, whose characteristic polynomial is $Ch(G_4) = x^4 - 4\ x^2 - 2\ x + 1$.



j	G_4-e_j	$Ch(G_4-e_j)$
1		$(x)(x^3 - 3\ x - 2)$
2,3		$x^4 - 3\ x^2 + 1$
4		$x^4 - 3\ x^2$

$$\sum_{j=1}^{4} Ch(G_4 - e_j) = 4\ x^4 - 12\ x^2 - 2\ x + 2$$

$$Ch(G_4) = (4/4)\ x^4 - (12/3)\ x^2 + (2/2) - (2/1)\ x$$

Proofs

Instead of Proposition 1 we shall verify a more general statement, namely Proposition 3. This result has been first deduced by Farrell and Wahid[8]. Nevertheless we will reproduce the entire proof of Proposition 3 because its details are later needed in the proof of Proposition 2.

The matching polynomial of a graph G will be denoted by Ma(G). It is known[9] that

$$Ma(G) = \sum_{k=0}^{m} (-1)^k\ p(G,\ k)\ x^{n-2k} \tag{4}$$

i.e.

$$coef_{2k}\ Ma(G) = (-1)^k\ p(G,\ k)\ . \tag{5}$$

In the above equations p(G, k) denotes the number of selections of k independent (i.e. mutually non-incident) edges in the graph G.

If G is an acyclic graph, then its matching and charcteristic polynomials coincide[9]. Therefore Proposition 1 is an immediate consequence of the following

P r o p o s i t i o n 3. The matching polynomial of a graph G can be reconstructed from $Ma(G-e_j)$, $j=1,2,\ldots,m$ $(m \neq 2)$. Moreover,

$$\mathrm{coef}_{2k}\ \mathrm{Ma}(G) = \frac{1}{m-k}\ \mathrm{coef}_{2k} \sum_{j=1}^{m} \mathrm{Ma}(G-e_j)$$

for $k = o,1,\dots,m-1$, and

$$\mathrm{coef}_{2m}\ \mathrm{Ma}(G) = 0$$

except if $G = m\ P_2 \dot{+} (n-2m)\ P_1$.

P r o o f. The matching polynomials conform to the following two recursion relations[9]:

$$\mathrm{Ma}(G) = \mathrm{Ma}(G-e_j) - \mathrm{Ma}(G-(e_j)) \tag{6}$$

and

$$\mathrm{Ma}(G) = x\ \mathrm{Ma}(G-v_i) - \sum_j \mathrm{Ma}(G-(e_j)) \tag{7}$$

where $G-(e_j)$ denotes the subgraph obtained from G by deletion of the edge e_j and both incident vertices. The summation on the right-hand side of (7) goes over all edges e_j which are incident to the vertex v_i. In addition, the matching polynomial satisfies an identity[10] which is fully analogous to eq. (1), viz.:

$$\sum_{i=1}^{n} \mathrm{Ma}(G-v_i) = \mathrm{Ma}'(G) \quad . \tag{8}$$

Now, summing eq. (7) over all vertices v_i of G and bearing in mind (8), we get

$$n\ \mathrm{Ma}(G) = x\ \mathrm{Ma}'(G) - 2 \sum_{j=1}^{m} \mathrm{Ma}(G-(e_j)) \quad .$$

Because of (6),

$$n \; Ma(G) = x \; Ma'(G) - 2 \sum_{j=1}^{m} Ma(G-e_j) + 2 \, m \; Ma(G)$$

i.e.

$$\sum_{j=1}^{m} Ma(G-e_j) = (x/2) \; Ma'(G) + (m-n/2) \; Ma(G)$$

and because of (4),

$$\sum_{j=1}^{m} Ma(G-e_j) = \sum_{k=0}^{m} (-1)^k \; (m-k) \; p(G, k) \; x^{n-2k} \; . \qquad (9)$$

Proposition 3 and therefore also Proposition 1 follow now by combining (9) and (5).

Proof of Proposition 2. If G is a monocyclic graph and C is its cycle, then[11]

$$Ch(G) = Ma(G) - 2 \; Ma(G-C) \quad . \qquad (10)$$

If the graph G has n vertices, then the subgraph G-C has $n-r$ vertices. Hence the number of vertices of G and G-C have opposite parity. Then as a consequence of (4), for all $k \geq 0$

$$coef_{2k} \; Ch(G) = coef_{2k} \; Ma(G) \qquad (11)$$

and

$$coef_{r+2k} \; Ch(G) = - \; 2 \; coef_{2k} \; Ma(G-C) \quad . \qquad (12)$$

If (10) holds and e_j is an edge of G, then also the following recursion relation is valid

$$Ch(G-e_j) = Ma(G-e_j) - 2 \; Ma(G-e_j-C) \quad . \qquad (13)$$

If e_j is an edge of the cycle C, then $G-e_j$ is an acyclic graph. Consequently, it is not possible to delete the cycle C from $G-e_j$ and the symbol $G-e_j-C$ is meaningless. In order to maintain the validity of eq. (13) we have to assume that $Ma(G-e_j-C) \equiv 0$ whenever e_j is an edge of C. Then (13) holds for all edges e_j of the graph G.

For similar reasons we have to define $Ma(G-C-e_j) \equiv 0$ if the subgraph G-C does not contain the edge e_j.

Hence if e_j is an edge of the cycle C,

$$Ma(G-e_j-C) = Ma(G-C-e_j) \equiv 0 \ . \qquad (14)$$

If e_j is an edge of G which is independent of the cycle C, then

$$Ma(G-e_j-C) = Ma(G-C-e_j) \ . \qquad (15)$$

If, finally, e_j is an edge of G which is incident to the cycle C (but does not belong to it), then

$$Ma(G-e_j-C) = Ma(G-C) \qquad (16\ a)$$

whereas

$$Ma(G-C-e_j) \equiv 0 \ . \qquad (16\ b)$$

Taking into account relations (14)-(16) we conclude that

$$\sum_{j=1}^{m} Ma(G-e_j-C) = \sum_{j=1}^{m} Ma(G-C-e_j) + m_i\ Ma(G-C) \ , \qquad (17)$$

where m_i is the number of edges of G which are incident to C.

If m_o is the number of edges of the graph G-C, then it is easy to see that $m_o + m_i + r = m$.

We are now prepared to deduce eqs. (2) and (3). In order to do this we have to sum the identity (13) over all edges of G. Since the subgraphs $G-e_j$ and $G-e_j-C$ have n and n-r vertices, respectively, according to (11) and (12) we have

$$\mathrm{coef}_{2k} \sum_{j=1}^{m} \mathrm{Ch}(G-e_j) = \mathrm{coef}_{2k} \sum_{j=1}^{m} \mathrm{Ma}(G-e_j) \tag{18}$$

and

$$\mathrm{coef}_{r+2k} \sum_{j=1}^{m} \mathrm{Ch}(G-e_j) = -2\ \mathrm{coef}_{2k} \sum_{j=1}^{m} \mathrm{Ma}(G-e_j-C)\,. \tag{19}$$

Eq. (2) follows now by applying Proposition 3 to (18).

Combining (19) with (17) and then applying Proposition 3 we get

$$\mathrm{coef}_{r+2k} \sum_{j=1}^{m} \mathrm{Ch}(G-e_j) = -2(m_o - k)\ \mathrm{coef}_{2k}\ \mathrm{Ma}(G-C) -$$

$$- 2\ m_i\ \mathrm{coef}_{2k}\ \mathrm{Ma}(G-C) = -2(m-r-k)\ \mathrm{coef}_{2k}\ \mathrm{Ma}(G-C)\ .$$

Eq. (3) follows now because of the relation (12).

This completes the proof of Proposition 2.

Proposition 2 can be extended in the following manner. If G is a polycyclic graph whose all cycles are odd, have equal size and no two of them are independent, then Ch(G) can be reconstructed from $\mathrm{Ch}(G-e_j)$, $j=1,2,\ldots,m$. For other polycyclic graphs the reconstruction problem remains unsolved.

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