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Characteristic polynomials of large graphs. On alternate form of characteristic polynomial [1]

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A recursion exists between the absolute magnitudes of the coefficients of the characteristic polynomials of certain families of cyclic and acyclic graphs which makes their computation quite easy for very large graphs using a pencil-and-a-paper approach. Structural requirements are given for such families of graphs which are of interest to the problem of recognition defined in [1].

Key words: Characteristic polynomial—acyclic polynomial—cycle polynomial

1. Introduction

Recently Randić [1] wrote an interesting paper on an alternate representation of characteristic polynomials, $P(G, x)$'s of certain families of graphs in terms of L_n, the characteristic polynomial of a paths on n vertices.

The purpose of this communication is to cite an observation on a recurrence relation occurring between the absolute magnitudes of the coefficients of $P(G, x)$'s of certain families of cyclic and acyclic graphs. Identifying such a relation allows construction of $P(G, x)$'s of very large graphs feasibly without resort to a computer.

2. Notation

We shall resolve characteristic polynomial into acyclic and cycle parts, thus

$$P(G, x) = P^{ac}(G, x) + P^{cy}(G, x) \tag{1a}$$

$$\sum_{m=0}^{n} a_m x^{n-m} = \sum_{m=0}^{n} a_m^{ac} x^{n-m} + \sum_{m=0}^{n} a_m^{cy} x^{n-m} \tag{1b}$$

where n is number of vertices in G. The first terms in Eqs. (1a) and (1b) correspond to the acyclic polynomial [2] while the second terms will be called here *cycle* polynomials [3]. They arise from Sachs graphs [4] containing *at least* one cycle, thus

$$a_m^{cy} = \sum_{s \in S_m^{cy}} (-1)^{c(s)} 2^{r(s)} \tag{2a}$$

$$a_m^{ac} = \sum_{s \in S_m^{ac}} (-1)^{(s)} \tag{2b}$$

S_m^{cy} is a Sachs graph on m vertices which contains at least one cycle while S_m^{ac} is an acyclic Sachs graph, $c(s)$ is, as usual, number of components and $r(s)$ number of cycles in the relevant Sachs graph.

3. Results

The families of graphs presented in Randić's paper [1] obey one or more of the following types of recursions: (G_n is a graph on n vertices)

$$|a_i^{ac}(G_n)| + |a_{i+2}^{ac}(G_{n+1})| = |a_{i+2}^{ac}(G_{n+2})| \qquad i = 0, 2, 4, \ldots. \tag{3a}$$

$$|a_i^{cy}(G_n)| + |a_{i+2}^{cy}(G_{n+1})| = |a_{i+2}^{cy}(G_{n+2})| \tag{3b}$$

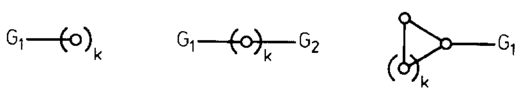
$i = 0, 2, 4, \ldots$ and $i = 3, 5, 7, \ldots$ (a_1 is always equal to zero)

where in general $|a_j(G_n)|$ is the absolute magnitude of the jth coefficient of G_n. For acyclic structures (3b) does not exist and $a_i^{ac}(G_m) = a_i(G_m)$ i.e. characteristic and acyclic polynomials coincide and the superscripts may be dropped, thus:

$$|a_i(G_n)| + |a_{i+2}(G_{n+1})| = |a_{i+2}(G_{n+2})| \qquad i = 0, 2, 4, \ldots \tag{3c}$$

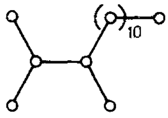
Eq. (3c) also holds for families of cyclic structures containing no odd cycles (see later).

We shall treat three types of families presented in Ref. [1], viz.,



(I) (II) (III)

where G_1 and G_2 may or may not be identical and may be cyclic or acyclic graphs. E.g. the first set in Table 2, [1], corresponds to type (I) with $G_1 =$  and $k = 0, 1, 2, 3, 4$, respectively. Similarly the fifth set of graphs of Table 2, (1), corresponds to type (II) with $G_1 = G_2 =$  with $k = 0, 1, 2, 3$ respectively. The two sets in Table 7, (1), correspond to type (I) where $G_1 = C_3$ and C_4 respectively and $k = 1, 2, 3, 4, 5$. The sets of graphs shown in Table 8, [1], belong to (III) with $k = 1, 2, 3, 4, 5$. We state the following observations: (1) when G_1 and G_2 are both acyclic graphs Eq. (3c) applies. E.g. $P(T_{16,x})$ might easily be calculated

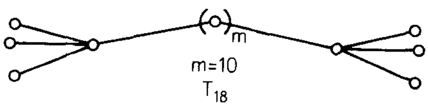


T_{16}

From $P(T, x)$'s of the first two trees in the last set of Table 2, [1] and eight applications of recurrence (3c), thus

$$P(T_{16}, x) = x^{16} - 15x^{14} + 89x^{12} - 266x^{10} + 422x^{8} - 343x^{6} + 123x^{4} - 12x^{2}$$

Similarly to compute $P(T_{18}, x)$, we have to know only



T_{18}

$P(T, x)$'s of the first two members: the absolute magnitudes of the a's are listed below:

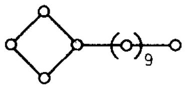
m								
1	1	8	15					
2	1	9	22	9				
3	1	10	30	24				
10	1	17	114	381	658	546	172	9

(2) For types (I) and (II) in which G_1 and/or G_2 are even-membered cycles, recursions (3a) and (3b), with i being even integers, apply: and whence, also, recurrence (3c). The second set of Table 7, [1], illustrates this case, the absolute magnitudes of their cyclic and acyclic coefficients are listed below:

a_4^{cy}	a_6^{cy}	a_8^{cy}
2	0	0
2	2	0
2	4	0
2	6	2
2	8	6

a_0^{ac}	a_2^{ac}	a_4^{ac}	a_6^{ac}	a_8^{ac}
1	5	4	0	
1	6	8	2	0
1	7	13	6	0
1	8	19	14	2
1	9	26	27	8

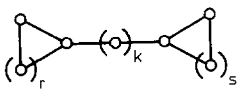
Knowing the signs (which is trivial) we can compute the a'_{js}. Thus, e.g. $P(G_{14}, x)$ might most easily be computed; it is:



G_{14}

$$P(G_{14}, x) = x^{14} - 14x^{12} + 74x^{10} - 184x^{8} + 271x^{6} - 106x^{6} + 14x^{2}.$$

The method is *not* restricted to cyclic graphs with pending bonds [5]. Relation (3c) applies to a homologous series of graphs containing *even-membered rings of constant size throughout the series.* As an illustration, we consider the series



G(r,s)
k=0, 1, 2, ...

The cyclic coeffizients are (for r=2, s=4)

k	a_4^{cy}	a_6^{cy}	a_8^{cy}	a_{10}^{cy}	a_{12}^{cy}
0	-2	10	-10	4	0
1	-2	12	-16	6	0
2	-2	14	-26	16	-4
⋮					

The acyclic coeffizients are:

k	a_0^{ac}	a_2^{ac}	a_4^{ac}	a_6^{ac}	a_8^{ac}	a_{10}^{ac}	a_{12}^{ac}
0	1	-11	41	-61	32	-4	0
1	1	-12	51	-92	66	-14	0
2	1	-13	62	-133	127	-46	4
⋮							

And since $a_i = a_i^{ac} + a_i^{cy}$, i even, we have an easy pencil-and-a-paper method for constructing $P(G, x)$'s for very large cyclic graphs (of course the series might be expanded as we please).

(3) For types (I), (II) in which either (or both) rings are odd-membered, contributions from cyclic Sachs graphs on odd vertices do not vanish, and hence their $P(G, x)$'s contain contributions from odd coefficients. In such cases recurrence relations 3a and 3b (with i both odd and even) hold. For $r = s = 1$, we obtain the

following quantities:

Cyclic coefficients
Odd subscripts

k	a_3^{cy}	a_5^{cy}	a_7^{cy}	a_9^{cy}
1	-4	16	-4	0
2	-4	20	-16	0
3	-4	24	-32	4
⋮				

Even subscripts

k	a_6^{cy}	a_8^{cy}
1	4	0
2	4	-4
3	4	-8
⋮		

Acyclic coefficients

k	a_0^{ac}	a_2^{ac}	a_4^{ac}	a_6^{ac}	a_8^{ac}
1	1	-8	17	-6	0
2	1	-9	24	-17	1
3	1	-10	32	-34	7
⋮					

Thus the coefficients of the characteristic polynomials are:

k	a_0	a_2	a_3	$-a_4$	a_5	a_6	a_7	a_8	a_9
1	1	-8	-4	17	16	-2	-4	0	0
2	1	-9	-4	24	20	-13	-16	-3	0
3	1	-10	-4	32	24	-30	-32	-1	4

We observe that recurrence relation holds only for *odd subscripted coefficients of their* $P(G, x)$*'s* i.e. Eq. (3c) with $i = 3, 5, 7, \ldots$. This presents no difficulty, however, since both Eqs (3a) and (3b) hold for the "*resolved parts*" of $P(G, x)$. To illustrate this subtle point we list a_6 and a_8 for the above family *resolved* as follows:

k	a_6^{cy}	+ a_6^{ac}	a_8^{cy}	+ a_8^{ac}
1	4	-6		
2			-4	+1
3			-8	+7

→

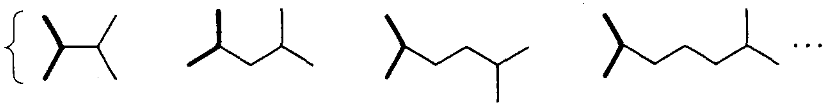
a_6	a_8
-2	
	-3
	-1

The above picture is symptomatic for graphs of type $G(r, s)$ where either r and/or s being an odd integer. We might easily expect Eq. (3c) with $i = 3, 5, 7$ to hold for the upper family of graphs shown in Table 7, [1], and (3c), $i = 0, 2, 4, \ldots$ to hold for the second set of graphs.

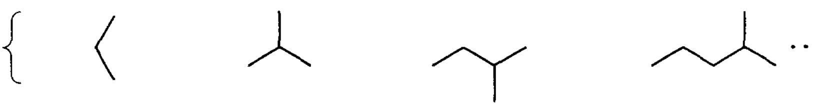
(4) For graphs of type III, examples of which are given by the three families of graphs shown in Table 8, it might be shown that *only* recursion (3a) holds.

Conjecture

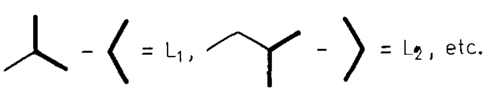
Let G_n be a graph on n vertices and $\{G_n, G_{n+1}, G_{n+2}, \ldots, G_\infty\}$ be a homologous family of graphs. Let g be a common subgraph in the set (where g may be an empty graph). The family $\{G'_n, G'_{n+1}, \ldots, G'_\infty\}$ results when g is pruned out of all members. Now we form all graphs $\{G'_{ij}\}$ where $G'_{ij} = G'_i - G'_j$ for all $i > j$, with $i \leq n$. If, then all G'_{ij}'s are *paths*, one or more of recursions (3a–3c) hold depending on cyclic and acyclic structures present (c.f. cases 1–4 above). E.g. consider the fifth set in Table 2, [1], viz.



where $g =$  , thus the primed family is



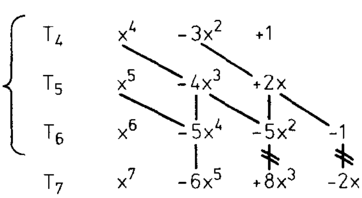
we observe that all G'_{ij}'s are paths, e.g.



As a further illustration we consider the following set of trees (which are transformable into benzenoid graphs whose sextet polynomials are identical to the $P(T, x)$'s, [6])

T_4 T_5 T_6 T_7

Let $g = \varnothing$ (an empty subgraph), then we have $T_5 - T_4 = T_6 - T_5 = T_7 - T_6 = L_1$; $T_6 - T_4 = L_2$, but $T_7 - T_5 = L_1.L_1$, a disconnected graph and thus we should *not* expect T_7 to obey (3a), indeed it does not: the $P(T, x)$'s are:



Conclusion

All graphs might in principle be regressed down to very small graphs if we recognize a *family* for every graph. By repeated use of recursions type 3 one

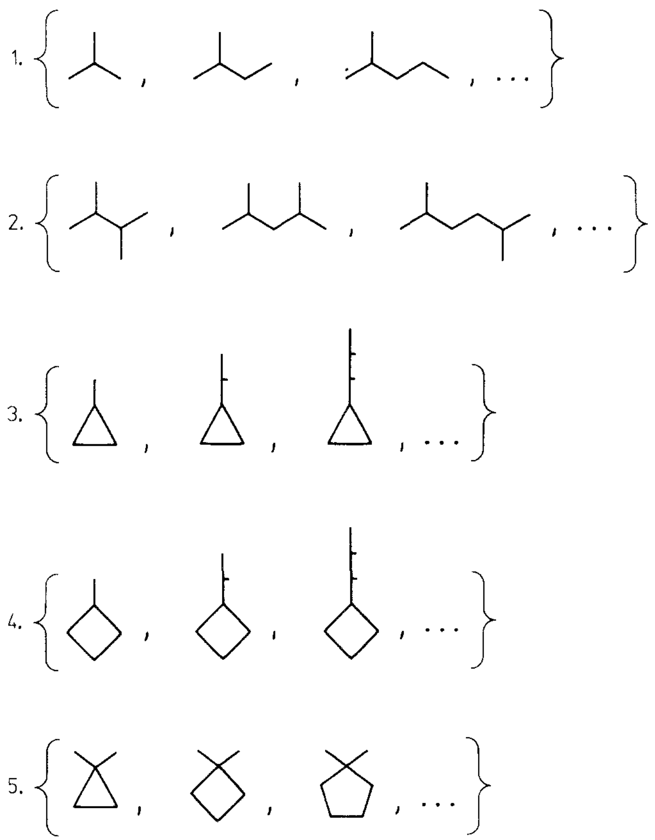


Fig. 1. Some representative graphs studied in this work reproduced from Ref. [1]. Sets 1, 2 are from Table 2, sets 3, 4 from Table 7 while set 5 is taken from Table 8. Sets 1, 3, 4 represent type I, set 2 represents type II and set 5 represents type III of graphs studied here

obtains polynomials for potentially very large graphs. The *resolution* of $P(G, x)$'s into cyclic and acyclic parts clarifies possible recursions existing between polynomial coefficients.

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