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A NOTE ON SOME COEFFICIENTS OF THE CHEBYSHEV POLYNOMIAL FORM OF THE CHARACTERISTIC POLYNOMIAL

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Abstract

The characteristic polynomial of a graph, which traditionally is written down in descending powers of X, can also be expressed in the mathematically equivalent form of a linear combination of the characteristic polynomials of linear chains, and often this expression is a simpler one. Investigation of the first few coefficients reveals that in this form the even ones are of smaller magnitude because they are more closely related to the cyclomatic number of the graph. On the other hand, the early odd coefficients are the same or are more complicated in composition.

1. Introduction

The characteristic polynomial is a well-known graph invariant that has a number of applications. For a graph of n vertices, it is commonly defined as $(-1)^n \cdot |A - XI|$, where A is an adjacency matrix, and I the unit matrix. References [1–22], selected from many, give an introduction to the nature and properties of this polynomial.

The coefficients of X^i $(i = 0 \ldots n)$ can in principle be evaluated by counting appropriate subgraphs [3], although in practice this is a tedious and unwieldy procedure if there are more than a few vertices (atoms) and, judging by the sparsity of published computer-oriented algorithms using this method, it is one that is not easily mechanised.

The relationship between these coefficients and certain subgraphs means that some properties of a given graph can be deduced by inspecting its characteristic polynomial alone, although it contains less information (for more than one graph may have the same characteristic polynomial). In general though, it is difficult to reconstruct a graph, or set of isospectral graphs, from a given arbitrary characteristic polynomial.

When it is possible to interpret a particular coefficient in terms of rather simple structural features than can readily be perceived in a graph, it becomes of interest as, for example, a potential topological index or a concise storage code for selected information. With the exception of the final term, which in certain cases gives just the algebraic structure count [12], this tends to become more difficult as the exponent of X decreases. General results for the terms in $X^n \ldots X^{n-4}$ (coefficients $a_0 \ldots a_4$) have been reported [6–8,12,14,16,20–22] and a few others of restricted validity. Among the best known relationships are that the value of a_1 equals the sum of any vertex weights; that $-a_2$ gives the number of edges of an unweighted graph; and that $-a_3/2$ gives the number of 3-membered rings present [12].

An alternative, and mathematically equivalent, way of expressing a characteristic polynomial is as a linear combination of the characteristic polynomials of linear chains. These are each denoted by L_i ($i = 0 \ldots n$ for an n vertex system), and are Chebyshev polynomials in $X/2$. This notation is useful and economic, and has been in occasional use for many years (e.g. [13,15,19,23–27]). The two schemes may be exemplified by butadiene ($CP = X^4 - 3X^2 + 1$ or L_4) and cyclobutadiene ($CP = X^4 - 4X^2$ or $L_4 - L_2 - 2$).

These L_i terms are often observed to have coefficients which are smaller than those of the corresponding X^i terms. The information contained in the polynomial as a whole must be the same no matter how the polynomial is expressed, but its distribution can differ. The general topological dependency of this form has been analysed and commented on [25]. This paper briefly examines a possible interpretation of some of the L_i coefficients, particularly in the light of recent work by Dias on the traditional characteristic polynomial [16,20- 22]. It should be noted, however, that the L_i notation does not always give a simpler expression [28].

Although for manipulative purposes a graph and its characteristic polynomial can often be treated interchangeably, it is as well here to make a distinction. The Chebyshev expansion provides an alternative way of viewing the structure of the polynomial: as a combination of L_i terms, each representing the characteristic polynomial of a chain. However, whereas the sum of two polynomials has an obvious meaning, a sum of two graphs does not. This is in contrast to a *product* of characteristic polynomials or of graphs, where neither concept causes difficulty (the latter is a disconnected graph).

It follows that reformulation of a characteristic polynomial in terms of its Chebyshev expansion does not in itself help to illuminate a structure in the same way that, say, a knowledge of how many 3-membered rings are present does. (It may, on the other hand, be useful as a means of comparing and classifying structures and their relationships.) The question considered here is why the L_i coefficients are often smaller than those of X^i, and whether they are any more or less useful. In fact, it is found that the relative simplicity of some even coefficients in the L_i form arises because in each case some "cancelling out" of edges and vertices through Euler's relationship occurs, so giving numbers which are related more intimately to a ring count than to edge or vertex counts. Apart from this heavy and repeated dependence on the ring total, the coefficients investigated here do not provide fresh information.

2. Results

The two forms of the characteristic polynomial can be written as

$$X^n + a_1 \cdot X^{n-1} + a_2 \cdot X^{n-2} + a_3 \cdot X^{n-3} + \ldots + a_{n-1} \cdot X + a_n$$

and

$$L_n + z_1 \cdot L_{n-1} + z_2 \cdot L_{n-2} + z_3 \cdot L_{n-3} + \ldots + z_{n-1} \cdot L_1 + z_n .$$

The coefficients of X^n and L_n are always 1 by definition, and the values of X^0 and L_0, which are not shown, are also 1.

Each L_i term in the L_n sequence refers to the characteristic polynomial of a chain, which has the known form [2]:

$$L_n = \sum_{m=0}^{n/2} (-1)^m \binom{n-m}{m} X^{n-2m} .$$

Pairs of coefficients (a_i and z_i) can be related by expanding terms in the L_n expression and summing like powers of X. From the fact that L_n has by definition no term in X^{n-1}, it follows that $z_1 = a_1$, and so

$$z_1 = \text{sum of vertex weights, if any.} \tag{1}$$

The two forms of the 2nd coefficient can be related by the equation $z_2 = a_2 - b_2$, where b_2 is the 2nd coefficient of L_n, and a_2 is known to be minus (number of edges) [6,12]. Thus, z_2 (in agreement with ref. [25]) gives a ring count [29] rather than an edge count for the graph (the expression has additional terms if weighted edges are present [12]):

$$z_2 = -R \text{ (where } R \text{ is the cyclomatic number [29]).} \tag{2}$$

For the 3rd coefficient, if no vertex is weighted, the two coefficients z_3 and a_3 are identical, and give the number of 3-membered rings. Otherwise, a second term is present:

$$z_3 = z_1 \cdot (n-2) - 2r_3 . \tag{3}$$

For the 4th coefficient of an unweighted system, use of Dias' recent formula [16],

$$a_4 = (q^2 - 9q + 6n)/2 - 2r_4 - v_1 - v_4 - 3v_5 - 6v_6 - 10v_7 - \ldots$$

(q = no. of edges; v_i = no. of vertices of valency i; r_4 = no. of 4-membered rings present) gives

$$z_4 = [(R-1)(R-4)]/2 - 2r_4 - v_1 - v_4 - 3v_5 - 6v_6 - 10v_7 - \ldots \quad (4)$$

By comparing the term $[(R-1)(R-4)]/2$ with $[q^2 - 9q + 6n]/2$, it can be seen that the L_4 coefficient will be smaller than a_4 for a given system size. The expression $[(R-1)(R-4)]/2$ provides no new information and can be evaluated as $[(z_2+1)(z_2+4)]/2$, constant for a given number of rings, and equal to 2 for all trees. As with a_4, among trees of maximum valency 4, z_4 depends only upon the number of vertices of degree 1 and 4.

The 5th coefficient a_5 is related to the number of 3- and 5-membered rings present, but does not appear to have been written in a completely general form [21]. Summing appropriate coefficients gives

$$z_5 = a_5 + 2r_3(4-n) + z_1(n^2 - 5n + 4)/2, \quad (5)$$

which differs from a_5 only in information repeated from earlier coefficients.

There is no general formula for a_6, but

$$a_6 = -(q^3 - 27q^2 + 146q + 36)/6 - n(3q - 22) - n_0 - 2r_6$$

for benzenoids [16],

where r_6 gives the number of hexagons and n_0 the number of bay regions. From this

$$z_6 = -(R^3 - 15R^2 + 80R)/6 - (n+3) - n_0 \text{ for benzenoids.} \quad (6)$$

So for this type of structure, the principal difference between the two forms is that the cubic function within z_6 relates to the ring count, whilst in a_6 it is to the edge count, so that z_6 is smaller and easier to evaluate.

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References

[1] C.A. Coulson, Proc. Cambridge Phil. Soc. 46(1950)202.

[2] L. Collatz and U. Sinogowitz, Abhandlungen Math. Seminar, Universität Hamburg 21(1957) 64.

[3] H. Sachs, Publ. Math. (Debrecen) 11(1964)119.

[4] L. Spialter, J. Chem. Doc. 4(1964)261; 269.

[5] H. Hosoya, Bull. Chem. Soc. Jap. 44(1971)2332.

[6] A. Graovac, I. Gutman, N. Trinajstić and T. Živković, Theor. Chim. Acta 26(1972)67.

[7] I. Gutman, Croat. Chem. Acta 46(1974)209.

[8] N. Trinajstić, Croat. Chem. Acta 49(1977)593.

[9] C.A. Coulson, B. O'Leary and R.B. Mallion, *Hückel Theory for Organic Chemists* (Academic Press, London, 1978).

[10] A.J. Schwenk and R.J. Wilson, in: *Selected Topics in Graph Theory,* ed. L.W. Beineke and R.J. Wilson (Academic Press, New York, 1978).

[11] D. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs – Theory and Application* (Academic Press, London, 1980).

[12] J.V. Knop and N. Trinajstić, Int. J. Quant. Chem. Symp. 14(1980)503.

[13] M. Randić, J. Comput. Chem. 3(1982)421.

[14] I. Gutman, J. Chem. Soc., Faraday Trans. 2, 79(1983)337.

[15] E.C. Kirby, J. Chem. Res. (S) (1984) 1.

[16] J.R. Dias, Theor. Chim. Acta 68(1985)107.

[17] P. Křivka, Ž. Jericević and N. Trinajstić, Int. J. Quant. Chem. Symp. 19(1985)129.

[18] M. Randić, J. Math. Chem. 1(1987)145.

[19] P. Křivka, R. B. Mallion and N. Trinajstić, Chemical graph theory VII. On Ulam subgraphs, J. Mol. Struct. (Theochem), in press. Preprint kindly supplied by Dr. R.B. Mallion, and references therein.

[20] J.R. Dias, J. Mol. Struct. (THEOCHEM) 149(1987)213.

[21] J.R. Dias, in: *Graph Theory and Topology in Chemistry,* ed. R.B. King and D.H. Rouvray, in press; and personal communication.

[22] J.R. Dias, Can. J. Chem. 65(1987)734.

[23] T.H. Goodwin and V. Vand, J. Chem. Soc. (1955) 1683.

[24] M. Randić, Theor. Chim. Acta 62(1983)485.

[25] H. Hosoya and M. Randić, Theor. Chim. Acta 63(1983)473.

[26] E.C. Kirby, Croat. Chem. Acta 59(1986)635.

[27] L. Grajcar et al., Theor. Chim. Acta 71(1987)299.

[28] E.C. Kirby, unpublished work.

[29] The enumeration of rings can sometimes be ambiguous [30]. Here, R refers to the smallest set of smallest rings, the "cyclomatic number" $(n - q + 1)$, and "r_i" refers to the number of i-membered rings. When a ring can be classified under both headings, it is counted twice.

[30] S.B. Elk, J. Chem. Inf. Comput. Sci. 24(1984)203; 25(1985)11; 25(1985)17; 27(1987)67; 27(1987)70.