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The use of Frame's method for the characteristic polynomials of chemical graphs

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The evaluation of characteristic polynomials of graphs of any size is an extremely tedious problem because of the combinatorial complexity involved in this problem. While particular elegant methods have been outlined for this problem, a general technique for any graph is usually tedious. We show in this paper that the Frame method for the characteristic polynomial of a matrix is extremely useful and can be applied to graphs containing large numbers of vertices. This method reduces the difficult problem of evaluating the characteristic polynomials to a rather simple problem of matrix products. The coefficients in the characteristic polynomial are generated as traces of matrices generated in a recursive product of two matrices. This method provides for an excellent and a very efficient algorithm for computer evaluation of characteristic polynomials of graphs containing a large number of vertices without having to expand the secular determinant of the matrix associated with the graph. The characteristic polynomials of a number of graphs including that of a square lattice containing 36 vertices are obtained for the first time.

Key words: Graph theory—characteristic polynomials—Frame's method for characteristic polynomials

1. Introduction

Chemists and mathematicians recognize the problem of evaluating characteristic polynomials of graphs to be a very difficult one. This is a consequence of the fact that the determinant expansion of large matrices is a cumbersome problem. Thus this problem has received considerable attention in the past few decades [1–34]. Chemists have shown considerable interest in characteristic polynomials of graphs for a number of reasons. Graphs are very useful in chemistry because they

represent interactions (quantum mechanical or statistical mechanical), lattices, NMR spin Hamiltonian [35], isomerizations, reaction networks and molecules themselves [36, 34]. The characteristic polynomial of a graph is an important structural invariant although it may not be a unique invariant in the sense different labelings of a structure lead to the same characteristic polynomial. Characteristic polynomials, spectra of graphs, spectral moments and random walks on lattices are intimately related. Consequently, the study of one problem leads to significant information on the other.

Characteristic polynomials play an important role in lattice statistics since they are useful in constructing matching polynomials which generate the number of possible ways of placing a given number of dimers on lattices.

Characteristic polynomials have played an important role in characterizing the aromaticity of polycyclic compounds. Characteristic polynomials of graphs facilitate the evaluation of matching polynomials used by Gutman, Trinajstić and others for aromatic compounds.

The characteristic polynomials of chemical graphs have significant applications in chemical kinetics [37], dynamics of oscillatory chemical reactions [14], solutions of Navier–Stokes equations [38] and several other applications in statistical mechanics.

The coefficients in the characteristic polynomials of molecular graphs are quite useful in evaluating several topological indices such as Hosoya index which are quite useful in correlating topological properties of molecules to their physical properties such as thermodynamic properties. One of the achievements of graph theory in this area is the characterization and construction of isospectral graphs. Although two graphs can be topologically inequivalent, they could have the same characteristic polynomial. Thus two isospectral molecules are expected to have similar properties in this model. Conversely, two molecules with different characteristic polynomials are expected to have different properties thus making it possible to relate molecules on the basis of their spectral differences.

Several papers have appeared which discuss methods for constructing characteristic polynomials of graphs. Most of these methods are restricted and often applicable to particular structures. When applied to those structures, these methods, of course, lead to significant simplifications. Nevertheless, these methods do not appear to be quite general.

The present author developed [25] a tree pruning method for characteristic polynomials of trees. This was further extended to structures with pending bonds by Balasubramanian and Randić [26]. This method, however, is applicable only to trees or structures with pending bonds. In this sense it is not completely general.

Randić [1] has recently shown the use of Cayley–Hamilton theorem for characteristic polynomials of graphs. This method reduces the problem of characteristic polynomials to evaluating all powers of the adjacency matrix and then evaluating

the coefficients in the characteristic polynomial as solutions to a set of linear equations. This method seems to be quite efficient for several graphs. However, this method is not easily applicable to structures or graphs that possess symmetry elements. One then needs to construct adjacency matrices in symmetry-adapted bases. Hosoya and Ohkami [11] have recently obtained recursive relations for a few polyhex structures. However, such relations are not unique for all structures and they cannot be easily obtained for general cases.

Several years ago Frame [39] presented a paper in a mathematical meeting which contains a useful algorithm for the evaluation of characteristic polynomial of any square matrix. The author became aware of this from the book of Dwyer [40] where the Frame method and several of its ramifications are discussed. It appears that workers in the areas of chemical graph theory do not seem to be aware of the Frame method. This method is extremely easy to use with a computer for any graph as we will show in this paper. The Frame method provides an excellent algorithm for evaluating the coefficients of characteristic polynomials based on the recursive matrix product of two matrices. One of the objectives of this paper is to show the use of the Frame method for the characteristic polynomial of any graph. In Sect. 2 we describe the Frame method and in Sect. 3 several applications to very complicated graphs of interest in Chemistry are presented.

2. The Frame method

Frame [39, 40] developed an excellent and efficient method for the characteristic polynomial of any matrix. This method provides a recursion formula for the characteristic equation as well as adjoint, determinant and inverse of a matrix. The difficult problem of obtaining the characteristic polynomial of a graph is thus reduced to a rather simple problem of evaluating trace and product of matrices in this method. We now describe this method.

Let A be a matrix of order n. Frame wrote down the characteristic equation corresponding to A in the following form.

$$|\lambda I - A| = \lambda^n - C_1\lambda^{n-1} - C_2\lambda^{n-2} \cdots - C_k\lambda^{n-k-1} \cdots - C_{n-1}\lambda - C_n = 0. \qquad (1)$$

The problem is to obtain the integral coefficients $C_1, C_2, \ldots$ in the characteristic equation. The minor of any element of $(\lambda I - A)$ cannot have a term with power greater than $n-1$ and therefore one can write the adjoint of $\lambda I - A$ as

$$\text{Adj}\,(\lambda I - A) = \lambda^{n-1}A_0 + \lambda^{n-2}A_1 + \cdots + \lambda^{n-k-1}A_k + \cdots + A_{n-1}. \qquad (2)$$

A_k's are matrices that can be used as undetermined multipliers. Using the fact that a matrix postmultiplied by its adjoint gives the determinant, the following identity can be obtained:

$$(\lambda I - A)\,\text{Adj}\,(\lambda I - A) = |\lambda I - A| I = \lambda^{n-1}(\lambda I - A)A_0 + \lambda^{n-2}(\lambda I - A)A_1 + \cdots + \lambda^{n-k-1}(\lambda I - A)A_k + \cdots + (\lambda I - A)A_{n-1}. \qquad (3)$$

Eq. (3) on simplification yields (4)

$$|\lambda I - A|I = \lambda^n A_0 + \lambda^{n-1}(-AA_0 + A_1) + \lambda^{n-2}(-AA_1 + A_2) + \cdots + (-AA_{n-1}). \tag{4}$$

Comparing (4) with (1) we obtain

$$\begin{aligned} A_0 &= I \\ A_1 &= AA_0 - C_1 I \\ A_2 &= AA_1 - C_2 I \\ &\vdots \\ A_k &= AA_{k-1} - C_k I \\ &\vdots \\ 0 &= AA_{n-1} - C_n I. \end{aligned} \tag{5}$$

Thus the matrices A_k's are recursively obtained. Further it can be shown that the trace of AA_{k-1} is given by

$$C_k = \frac{\text{trace}\,(AA_{k-1})}{k}. \tag{6}$$

Consequently, the coefficients C_k's are simply generated as the traces of matrices AA_{k-1}'s which are constructed recursively by simple matrix products.

The Frame method thus provides an excellent and a very efficient polynomial algorithm for the characteristic polynomial of any matrix and hence for a graph. This algorithm is described below.

Let A be the adjacency matrix of a graph. Construct the matrices B_k's as follows.

$$B_1 = A(A - C_1 I), \qquad C_1 = \text{tr}\, A \tag{7}$$

$$C_2 = \tfrac{1}{2}\,\text{tr}\, B_1 \tag{8}$$

$$B_2 = A(B_1 - C_2 I) \tag{9}$$

$$C_3 = \tfrac{1}{3}\,\text{tr}\, B_2 \tag{10}$$

$$\vdots$$

$$B_{n-1} = A(B_{n-2} - C_{n-1} I) \tag{11}$$

$$C_n = \frac{\text{tr}\, B_{n-1}}{n} \tag{12}$$

Thus the coefficients C_k's are generated recursively as traces of matrices. In the next section we provide several applications of this method to graphs of chemical interest.

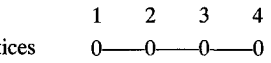


Fig. 1. A molecular graph containing four vertices

3. Application of the Frame method to characteristic polynomials of graphs

Let us consider the graph of butane as an example to illustrate the Frame method. The graph of butane is shown in Fig. 1. The adjacency matrix A is shown below

$$A=\begin{bmatrix}0&1&0&0\\1&0&1&0\\0&1&0&1\\0&0&1&0\end{bmatrix}$$

$$\operatorname{tr} A = C_1 = 0.$$

The matrices B_1, B_2 etc. are recursively constructed and shown below.

$$B_1=\begin{bmatrix}0&1&0&0\\1&0&1&0\\0&1&0&1\\0&0&1&0\end{bmatrix}\begin{bmatrix}0&1&0&0\\1&0&1&0\\0&1&0&1\\0&0&1&0\end{bmatrix}=\begin{bmatrix}1&0&1&0\\0&2&0&1\\1&0&2&0\\0&1&0&1\end{bmatrix}$$

$$C_2=\tfrac{1}{2}\operatorname{tr} B_1=3 \tag{12}$$

$$B_2=\begin{bmatrix}0&1&0&0\\1&0&1&0\\0&1&0&1\\0&0&1&0\end{bmatrix}\begin{bmatrix}-2&0&1&0\\0&-1&0&1\\1&0&-1&0\\0&1&0&-2\end{bmatrix}=\begin{bmatrix}0&-1&0&1\\-1&0&0&0\\0&0&0&-1\\1&0&-1&0\end{bmatrix}$$

$$C_3=\tfrac{1}{3}\operatorname{tr} B_2=0 \tag{13}$$

$$B_3=\begin{bmatrix}0&1&0&0\\1&0&1&0\\0&1&0&1\\0&0&1&0\end{bmatrix}\begin{bmatrix}0&-1&0&1\\-1&0&0&0\\0&0&0&-1\\1&0&-1&0\end{bmatrix}=\begin{bmatrix}-1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}$$

$$C_4=\tfrac{1}{4}\operatorname{tr} B_3=-1 \tag{14}$$

Thus the characteristic polynomial of the graph in Fig. 1 is

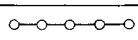
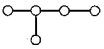
$$\lambda^4-3\lambda^2+1. \tag{15}$$

Consequently, the problem of evaluating the characteristic polynomial of a graph is reduced to a simple problem of recursive matrix products which can be handled very efficiently with the help of computers.

We have written a computer program based on the above method for evaluating the characteristic polynomial of any graph. The details of this program and other applications will be published in a future paper.

We present here the characteristic polynomials of several graphs obtained using the Frame method. Table 1 shows 8 graphs containing five vertices and their

Table 1. Characteristic polynomials of eight connected graphs containing five vertices obtained using Frame's method

Graph	Characteristic polynomial
	$\lambda^5 - 4\lambda^3 + 3\lambda$
	$\lambda^5 - 4\lambda^3 + 2\lambda$
	$\lambda^5 - 4\lambda^3$
	$\lambda^5 - 5\lambda^3 - 2\lambda^2 + 3\lambda$
	$\lambda^5 - 5\lambda^3 + 2\lambda$
	$\lambda^5 - 5\lambda^3 + 5\lambda - 2$
	$\lambda^5 - 6\lambda^3 - 2\lambda^2 + 4\lambda$
	$\lambda^5 - 6\lambda^3 - 4\lambda^2 + 3\lambda + 2$

characteristic polynomials. These results can be checked with available results for some of these graphs. For one of the graphs in that table we provide the intermediate matrices and their traces in Table 2 to illustrate the Frame method.

We now consider more complicated graphs whose characteristic polynomials cannot be easily obtained with other methods. Consider the Petersen graph in Fig. 2 and the isomerization graph of a tetrahedral pyramidal complex in Fig. 3. Both these graphs have been considered by Randić and co-workers [41] and their properties have been discussed by these authors in great detail. We applied the Frame method for these two graphs. The characteristic polynomials of these 2 graphs and 19 other complicated graphs were evaluated in only 7 seconds by our computer program. The characteristic polynomial of the Petersen graph is given by (16)

$$\lambda^{10} - 15\lambda^8 + 75\lambda^6 - 24\lambda^5 - 165\lambda^4 + 120\lambda^3 + 120\lambda^2 - 160\lambda + 48. \tag{16}$$

The characteristic polynomial of the isomerization graph of the tetrahedral pyramidal complex (in Fig. 3) is given by (17)

$$\lambda^{15} - 30\lambda^{13} - 20\lambda^{12} + 345\lambda^{11} + 396\lambda^{10} - 1940\lambda^9 - 3120\lambda^8 + 5280\lambda^7 + 12160\lambda^6 - 4224\lambda^5 - 23040\lambda^4 - 8960\lambda^3 + 15360\lambda^2 + 15360\lambda + 4096. \tag{17}$$

Table 2. The intermediate steps involved in evaluating the coefficients of the characteristic polynomial of the second graph in Table 1 using the Frame method (for an explanation of the notation and method, see text)

A	$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}$	$C_1 = \operatorname{tr} A = 0$
B_1	$\begin{bmatrix} 1 & 0 & 1 & 0 & 1 \\ 0 & 3 & 0 & 1 & 0 \\ 1 & 0 & 2 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{bmatrix}$	$C_2 = \frac{1}{2} \operatorname{tr} B_1 = 4$
B_2	$\begin{bmatrix} 0 & -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -2 & 0 \\ 1 & 0 & -2 & 0 & 1 \\ 0 & -1 & 0 & 1 & 0 \end{bmatrix}$	$C_3 = \frac{1}{3} \operatorname{tr} B_2 = 0$
B_3	$\begin{bmatrix} -1 & 0 & 0 & 0 & -1 \\ 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 \\ -1 & 0 & 0 & 0 & -1 \end{bmatrix}$	$C_4 = \frac{1}{4} \operatorname{tr} B_3 = -2$
B_4	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	$C_5 = \frac{1}{5} \operatorname{tr} B_4 = 0$
	Char Poly $= \lambda^5 - 4\lambda^3 + 2\lambda$	

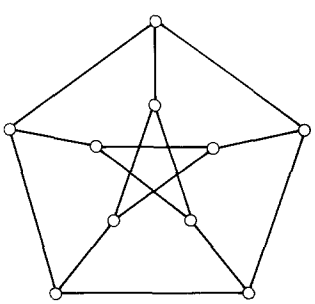


Fig. 2. The Petersen graph. For the characteristic polynomial of this graph, see expression (16)

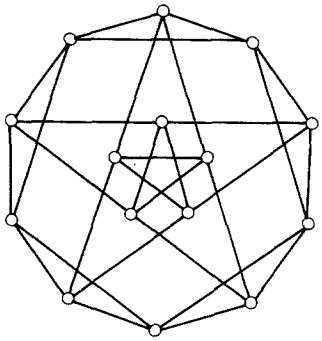


Fig. 3. The Isomerization graph of a tetrahedral pyramidal complex. For the characteristic polynomial of this graph, see expression (17)

We will consider two other periodic graphs that are of interest in aromaticity and related problems. Consider the graph in Fig. 4. This graph contains 24 vertices and thus the adjacency matrix of this graph is of order 24×24. Further because of a number of lines, the matrix has several non-zero elements. Consequently, the evaluation of the characteristic polynomial of this graph by determinant expansion and other methods is extremely difficult. The Frame method generates the characteristic polynomial of this graph very efficiently. The resulting polynomial is shown below.

$$\lambda^{24} - 30\lambda^{22} + 387\lambda^{20} - 2832\lambda^{18} + 13059\lambda^{16} - 39858\lambda^{14} + 82281\lambda^{12} - 115272\lambda^{10} + 108192\lambda^{8} - 65864\lambda^{6} + 24432\lambda^{4} - 4896\lambda^{2} + 400. \quad (18)$$

Note that the characteristic polynomial of the graph in Fig. 4 (expression 18) does not contain any term with odd power as expected.

Finally, consider the square lattice graph in Fig. 5. This is certainly a very complicated graph containing 36 vertices and consequently, all the other methods are not easily applicable to this problem. Our computer program generated the characteristic polynomial of this graph in 12 seconds. The characteristic polynomial of this graph is given by

$$\lambda^{36} - 60\lambda^{34} + 1572\lambda^{32} - 23{,}772\lambda^{30} + 231{,}126\lambda^{28} - 1{,}523{,}844\lambda^{26} + 7{,}005{,}754\lambda^{24} - 22{,}757{,}380\lambda^{22} + 52{,}393{,}405\lambda^{20} - 85{,}052{,}332\lambda^{18} + 96{,}104{,}022\lambda^{16} - 73{,}969{,}028\lambda^{14} + 37{,}486{,}225\lambda^{12} - 11{,}814{,}292\lambda^{10} + 2{,}074{,}464\lambda^{8} - 153{,}664\lambda^{6}. \quad (19)$$

The largest coefficient (i.e. the coefficient of λ^{16}) is of the order of 96 million which should explain the combinatorial complexity involved in this problem.

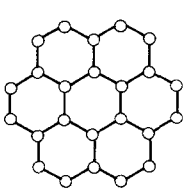


Fig. 4. A hexagonal lattice graph containing 24 vertices. The characteristic polynomial of this graph is given by expression (18)

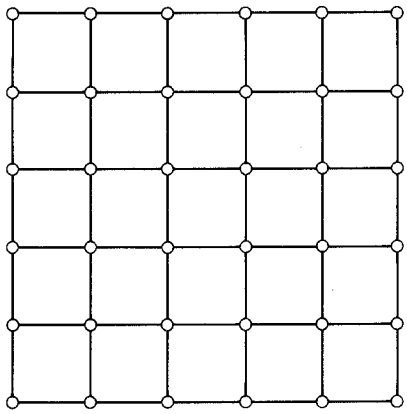


Fig. 5. A square lattice graph containing 36 vertices. The characteristic polynomial of this lattice is given by (19)

4. Conclusion

We have shown in this paper that the characteristic polynomial of many graphs (cyclic or acyclic) containing large numbers of vertices can be obtained using the Frame method. Thus the problem of the characteristic polynomial of graphs which is considered a very difficult problem is solved. The Frame method gives rise to a very elegant polynomial algorithm for this exponential problem and consequently computer program based on this method takes only a few seconds. We have written a computer program based on this method. The details of this program and further applications will appear in a future publication. Our program took only 35 seconds for a complicated hexagonal lattice graph containing 54 vertices. The largest coefficient in the characteristic polynomial of this graph is of the order of 2×10^{13} indicating the difficulty involved in evaluating this. In this paper examples of a number of complicated graphs were provided for which the characteristic polynomials were obtained easily using the Frame method!

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