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A NOTE ON THE CHARACTERISTIC POLYNOMIAL

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ABSTRACT

It is shown that the procedures of Le Verrier, Faddeev, and Frame for the computation of the characteristic polynomials represent the same method in three closely related formulations.

In the last few years, considerable attention has been given to the characteristic polynomial of a (chemical) graph.[1-5] The characteristic polynomial P(x) of a graph G is an important structural invariant. It is not unique because of the fact that non-isomorphic graphs may possess identical P(x)'s.[6,7] It is defined as det $|x\underline{I} - \underline{A}|$, where $\underline{A}$ and $\underline{I}$ are, respectively, the adjacency matrix of a graph G with N vertices and the unit matrix NxN.

The construction of the characteristic polynomial is tedious, because of the combinatorial complexity involved in the problem.[8] There are many techniques available for the generation of the characteristic polynomials of (complex) graphs: the expansion of the secular determinant,[9] matrix diagonalisation followed by the use of Viete formula,[10] direct graphical constructions,[1,11-15] the transfer matrix method,[16] the partition technique,[17] the polynomial matrix method,[18] the pruning technique,[19,20] the block-diagonalisation method,[21] the operator technique,[22] the Chebishev expansion,[23] the use of the Frobenius matrix,[24] and many more.

Recently Balasubramanian[4,25] has popularized the method of Frame[26] for the computation of the characteristic polynomial. Krivka et al.[27] have shown that the Frame method is similar to the Faddeev method,[28] which in turn represents a modification of the Le Verrier method.[29] The procedures of Le Verrier, Faddeev, and Frame are very general, and are efficient methods for bringing the secular equation into polynomial form. As such, they provide excellent algorithms for computer generation of the characteristic polynomial of (chemical) graphs. Because of this fact alone these procedures are worthy of further studies. In the present note we wish to report a detailed analysis of the relationship between the Le Verrier procedure, the Faddeev procedure, and the approach by Frame (as presented by Balasubramanian).

We first examine a property of the characteristic polynomial which, in terms of matrix algebra, is a generalization of the Bérout algebra theorem.[30]

Theorem 1 (a subsidiary theorem)

If

(i) $P(x) = x^N - a_1 x^{N-1} - a_2 x^{N-2} - \dots - a_{N-1} x - a_N$, **(1)**

(ii) $\underline{A}$ is a square $(N \times N)$ matrix,

(iii) $\underline{B}(x) = \underline{B}_o x^{N-1} + \underline{B}_1 x^{N-2} + \dots + \underline{B}_{N-2} x + \underline{B}_{N-1}$, **(2)**

where $\underline{B}_i$ $(i=0,1,\dots,N-1)$ are $(N\times N)$ matrices such that

$$(x\underline{I} - \underline{A})\, \underline{B}(x) = P(x)\, \underline{I}\,. \qquad \textbf{(3)}$$

Then,

$$P(\underline{A}) = \underline{0} \qquad \textbf{(4)}$$

Proof:

From eqs. (1), (2), and (3):

$$(x\underline{I} - \underline{A})(\underline{B}_o x^{N-1} + \underline{B}_1 x^{N-2} + \underline{B}_2 x^{N-3} + \dots + \underline{B}_{N-2} x + \underline{B}_{N-1}) =$$

$$= \underline{B}_o x^N - (\underline{A}\,\underline{B}_o - \underline{B}_1)\, x^{N-1} - (\underline{A}\,\underline{B}_1 - \underline{B}_2)\, x^{N-2} - \dots -$$

$$-(\underline{A}\,\underline{B}_{N-2} - \underline{B}_{N-1})\,x - \underline{A}\,\underline{B}_{N-1} = x^N\,\underline{I} - a_1 x^{N-1}\,\underline{I} - \ldots -$$

$$- a_{N-1}\,x\,\underline{I} - a_N\,\underline{I} \tag{5}$$

Comparison of the coefficients on the left- and right-hand sides of (5) gives

$$\underline{B}_o = \underline{I} \tag{6}$$

$$-(\underline{A}\,\underline{B}_o - \underline{B}_1) = -a_1\,\underline{I} \tag{7}$$

$$-(\underline{A}\,\underline{B}_1 - \underline{B}_2) = -a_2\,\underline{I} \tag{8}$$

$$-(\underline{A}\,\underline{B}_2 - \underline{B}_3) = -a_3\,\underline{I} \tag{9}$$

$$\vdots$$

$$-(\underline{A}\,\underline{B}_{N-2} - \underline{B}_{N-1}) = -a_{N-1}\,\underline{I} \tag{10}$$

$$-\underline{A}\,\underline{B}_{N-1} = -a_N\,\underline{I} \tag{11}$$

Multiplying eqs. (6) - (11) by $\underline{A}^N$, $\underline{A}^{N-1}, \ldots, \underline{A}$, $\underline{I}$ and adding, we obtain

$$\underline{A}^N\,\underline{B}_o - \underline{A}^{N-1}(\underline{A}\,\underline{B}_o - \underline{B}_1) - \underline{A}^{N-2}(\underline{A}\,\underline{B}_1 - \underline{B}_2) - \ldots -$$

$$- \underline{A}(\underline{A}\,\underline{B}_{N-2} - \underline{B}_{N-1}) - \underline{A}\,\underline{B}_{N-1} = \underline{A}^N - a_1\underline{A}^{N-1} - a_2\underline{A}^{N-2} - \ldots$$

$$- a_{N-1}\underline{A} - a_N\,\underline{I} = 0 \tag{12}$$

and eq. (4)

$$\underline{0} = P(\underline{A}) \tag{13}$$

We now introduce the Cayley-Hamilton theorem.[31]

Theorem 2 (Cayley-Hamilton theorem)

If $D(x)$ is the characteristic polynomial of the square $(N \times N)$ matrix $\underline{A}$, then

$$D(\underline{A}) = \underline{0} \tag{14}$$

Proof:

If $\underline{C}(x)$ is the inverse of a matrix $(x\,\underline{I} - \underline{A})$, then

$$(x\,\underline{I} - \underline{A})\ \underline{C}(x) = \underline{I}. \tag{15}$$

The matrix $\underline{C}(x)$ may be given in the form as follows

$$\underline{C}(x) = \frac{1}{\det |x\,\underline{I} - \underline{A}|}\ \underline{F}(x) \tag{16}$$

where $\underline{F}(x)$ is the adjoint matrix of $(x\,\underline{I} - \underline{A})$. Since the minor of any element of $(x\,\underline{I} - \underline{A})$ cannot have a term without a power greater than N-1, one can give the adjoint matrix $\underline{F}(x)$ in terms of eq. (2). The comparison of eqs. (15) and (16) produces

$$(x\,\underline{I} - \underline{A})\ \frac{\underline{F}(x)}{\det |x\,\underline{I} - \underline{A}|} = \underline{I} \tag{17}$$

Introducing

$$\det |x\,\underline{I} - \underline{A}| = D(x) \tag{18}$$

into (17), we obtain

$$(x\,\underline{I} - \underline{A}) \cdot \underline{F}(x) = D(x) \cdot \underline{I} \tag{19}$$

and by means of Theorem 1

$$D(\underline{A}) = \underline{0} \tag{20}$$

From these arguments we see that the Cayley-Hamilton theorem is a consequence of <u>Theorem 1</u>, when $P(x)$ is the characteristic polynomial of the matrix $\underline{A}$ and eqs. (6) - (11) still hold when $\underline{B}(x)$ is the adjoint matrix of $(x\,\underline{I} - \underline{A})$. From eqs. (6) - (11) we obtain the set of $\underline{B}$-matrices

$$\underline{B}_o = \underline{I} \tag{21}$$

$$\underline{B}_1 = \underline{A}\,\underline{B}_o - a_1\,\underline{I} \tag{22}$$

$$\underline{B}_2 = \underline{A}\,\underline{B}_1 - a_2\,\underline{I} \tag{23}$$

$$\vdots$$

$$\underline{B}_k = \underline{A}\,\underline{B}_{k-1} - a_k\,\underline{I} \tag{24}$$

$$\vdots$$

$$\underline{B}_{N-1} = \underline{A}\,\underline{B}_{N-2} - a_{N-1}\,\underline{I} \tag{25}$$

$$\underline{0} = \underline{B}_N = \underline{A}\,\underline{B}_{N-1} - a_N\,\underline{I} \tag{26}$$

After the elementary substitutions

$$\underline{A}_1 = \underline{A} \tag{27}$$

$$\underline{A}_2 = \underline{A}\;\underline{B}_1 \tag{28}$$

$$\vdots$$

$$\underline{A}_k = \underline{A}\;\underline{B}_{k-1} \tag{29}$$

$$\vdots$$

$$\underline{A}_{N-1} = \underline{A}\;\underline{B}_{N-2} \tag{30}$$

$$\underline{A}_N = \underline{A}\;\underline{B}_{N-1} \tag{31}$$

Equations (21) - (26) become

$$\underline{B}_1 = \underline{A}_1 - a_1 \underline{I} \qquad (32)$$

$$\underline{B}_2 = \underline{A}_2 - a_2 \underline{I} \qquad (33)$$

$$\vdots$$

$$\underline{B}_k = \underline{A}_k - a_k \underline{I} \qquad (34)$$

$$\vdots$$

$$\underline{B}_{N-1} = \underline{A}_{N-1} - a_{N-1} \underline{I} \qquad (35)$$

$$\underline{0} = \underline{B}_N = \underline{A}_N - a_N \underline{I} \qquad (36)$$

Combining eqs. (27) - (31) and (32) - (36) we obtain

$$\underline{A}_1 = \underline{A} \qquad (37)$$

$$\underline{A}_2 = \underline{A}^2 - a_1 \underline{A} \qquad (38)$$

$$\underline{A}_3 = \underline{A}^3 - a_1 \underline{A}^2 - a_2 \underline{A} \qquad (39)$$

$$\vdots$$

$$\underline{A}_k = \underline{A}^k - a_1 \underline{A}^{k-1} - a_2 \underline{A}^{k-2} - \dots - a_{k-1} \underline{A} \qquad (40)$$

Equating the traces of the matrices on the left- and right-hand sides of eqs. (37) - (40), a formula which coincides with the Newton formula[32] is obtained (The Newton formula allows one to obtain successive coefficients of the characteristic polynomial):

$$\mathrm{Tr}\, \underline{A}_k = \mathrm{Tr}\, \underline{A}^k - a_1 \mathrm{Tr}\, \underline{A}^{k-1} - a_2 \mathrm{Tr}\, \underline{A}^{k-2} - \dots -$$

$$- a_{k-1} \mathrm{Tr}\, \underline{A} = k \cdot a_k \qquad (41)$$

Thus,

$$a_k = \frac{1}{k}\,(\mathrm{Tr}\,\underline{A}^k - a_1\,\mathrm{Tr}\,\underline{A}^{k-1} - \ldots - a_{k-1}\,\mathrm{Tr}\,\underline{A}) \qquad (42)$$

or by means of (40)

$$a_k = \frac{1}{k}\,\mathrm{Tr}\,\underline{A}_k \qquad (43)$$

or by means of (29)

$$a_k = \frac{1}{k}\,\mathrm{Tr}\,\underline{A}\cdot\underline{B}_{k-1} \qquad (44)$$

We note that eq. (42) represents the master formula for computation of the coefficients in the Le Verrier method (also called the Cayley-Hamilton method)[2,33,34] and eq. (43) the master formula in the Faddeev method. Similarly, eq. (44) is the master formula for generation of the polynomial coefficients in the Frame method (as advocated by Balasubramanian). Since eqs. (42), (43), and (44) may be easily transformed amongst of themselves, all three of the above procedures reduce to the same method for the construction (and computation) of the characteristic polynomial.

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