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Characteristic polynomials of chemical graphs via symmetric function theory

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The characteristic polynomial corresponding to the adjacency matrix of a graph is constructed by using the traces of the powers of the adjacency matrix to calculate the coefficients of the characteristic polynomial via Newton's identities connecting the power sum symmetric functions and the elementary symmetric functions of the eigenvalues. It is shown that Frame's method, very recently employed by Balasubramanian, is nothing but symmetric functions and Newton's identities.

Key words: Characteristic polynomials — Chemical graphs — Symmetric function theory

1. Introduction

Many problems in graph theory that arise in organic chemistry eventually require the construction of the characteristic polynomial corresponding to the vertex adjacency matrix of the graph. The coefficients of the characteristic polynomial have an interpretation as sums of principal minors of the determinant of the adjacency matrix [1], although direct evaluation via this approach is feasible only for very small graphs. Collatz and Sinogowitz [2] were among the very first to study the relationship between the coefficients of the characteristic polynomial and the elements of the adjacency matrix by various techniques. Sachs [3], but see also Spialter [4] and Mowshowitz [5], showed that the coefficients of the characteristic polynomial are given by sums over various subgraphs. Trinajstic [6] has made extensive use of Sachs theorem to evaluate the characteristic polynomial of conjugated hydrocarbons. The monograph by Graovac, Gutman and Trinajstic [7], is a valuable source of information on this problem.

Since this manuscript was completed, two important papers have appeared: Balasubramanian [8] and Randic [9]. Each contains extensive references to the literature.

The purpose of this communication is to present a *general* procedure for constructing the characteristic polynomial. This procedure rests upon known properties of symmetric functions of the eigenvalues of the adjacency matrix, and employs the traces of the powers of the adjacency matrix to calculate the coefficients of the characteristic polynomial via Newton's identities connecting the power sum symmetric functions and the elementary symmetric functions.

2. The characteristic polynomial of the adjacency matrix

If G is an unoriented graph containing n vertices, then the adjacency matrix $\boldsymbol{A}(G)$ is a matrix of 0's and 1's such that [1]

$$A_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are adjacent vertices} \\ 0 & \text{if } i \text{ and } j \text{ are non-adjacent vertices.} \end{cases}$$

$\boldsymbol{A}$ is an $N \times N$ real, symmetric matrix and as such its eigenvalues are real. The set of all eigenvalues: $\lambda_1, \lambda_2, \ldots, \lambda_N$ is termed the graph spectrum and satisfies the characteristic polynomial

$$P(G; \lambda) = \det[\boldsymbol{A} - \lambda I]$$

$$= \sum_{n=0}^{N} (-1)^n p_n \lambda^{N-n}, \qquad p_0 \equiv 1. \tag{2.1}$$

The p_n are either integer-valued or zero. For example, $p_n \equiv 0$, when n is an odd integer, for alternant hydrocarbons [6]. As the size of the graph increases, the p_n become very large and numerical computations are probably best done in integer arithmetic (or in triple precision).

3. Construction of the characteristic polynomial

Central to our evaluation of the p_n are the traces of the powers of $\boldsymbol{A}$

$$\sigma_l \equiv \operatorname{tr} \boldsymbol{A}^l, \qquad l = 1, 2, \ldots, N. \tag{3.1}$$

Since $\boldsymbol{A}$ is symmetric, it can be diagonalized and the eigenvalues: $\lambda_1, \lambda_2, \ldots, \lambda_N$ form the principal diagonal. Obviously

$$\sigma_l = \sum_n \lambda_n^l. \tag{3.2}$$

Since the λ_n are real, so is σ_l. The σ_l are the power sum symmetric functions, see Bôcher [10] or Weyl [11]. The σ_l are invariant under the group of all $N!$ possible permutations of the N arguments. These permutations are linear transformations of the N-dimensional vector $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_N)$. The important point to note is that σ_l is obtained directly from $\boldsymbol{A}$ itself by raising $\boldsymbol{A}$ to the lth power and taking the trace, nowhere do we use the individual eigenvalues.

The p_n are the elementary symmetric functions formed from the eigenvalues. In the usual notation for elementary symmetric functions, see Bôcher [10] or Weyl [11]:

$$\begin{aligned} p_1 &= \sum \lambda_1 = \operatorname{tr} \boldsymbol{A} \\ p_2 &= \sum \lambda_1 \lambda_2 \\ p_3 &= \sum \lambda_1 \lambda_2 \lambda_3 \\ &\cdots \\ p_N &= \lambda_1 \lambda_2 \cdots \lambda_N = \det \boldsymbol{A}. \end{aligned} \tag{3.3}$$

The p_n are also invariant under the group of all $N!$ permutations of the N arguments.

Our problem is to express the p's in terms of the σ's. This is exactly the inverse of the problem that arises in the theory of equations where the p's are given and the σ's are to be evaluated, see Burnside and Panton [12].

The power sum symmetric functions and the elementary symmetric functions are related by Newton's identities [12]

$$\begin{aligned} &\sigma_n - \sigma_{n-1} p_1 + \sigma_{n-2} p_2 - \sigma_{n-3} p_3 + \cdots + (-1)^{n-2} \sigma_2 p_{n-2} \\ &\quad + (-1)^{n-1} \sigma_1 p_{n-1} + (-1)^n n p_n = 0 \end{aligned} \tag{3.4}$$

where $n \leq N$. We observe the convention that $p_n = 0$ if n is greater than the degree of the characteristic polynomial. Note that p_n is determined by $\sigma_1, \ldots, \sigma_n$; thus to evaluate p_5 (say) we require σ_1 to σ_5 only. Obviously p_N requires a knowledge of all σ's from σ_1 to σ_N.

Fortunately Newton's relations simplify even further because $\sigma_1 = 0$ (i.e. $\operatorname{tr} \boldsymbol{A} \equiv 0$), implying that $p_1 = 0$. Consequently Eq. (3.4) reduces to

$$\sigma_n + \sigma_{n-2} p_2 - \sigma_{n-3} p_3 + \cdots + (-1)^n n p_n = 0. \tag{3.5}$$

Thus given the σ's, we can generate the p's by recursion.

Although the p's are probably most easily obtained from the σ's by direct numerical evaluation of the Newton identities via computer, we list the first ten p_n as obtained by sequential manipulations for those who may require the explicit formulae:

$$2! p_2 = \sigma_2 \tag{3.6}$$

$$3! p_3 = 2\sigma_3 \tag{3.7}$$

$$4! p_4 = -6\sigma_4 + 3\sigma_2^2 \tag{3.8}$$

$$5! p_5 = 24\sigma_5 - 20\sigma_3\sigma_2 \tag{3.9}$$

$$6! p_6 = -120\sigma_6 + 90\sigma_4\sigma_2 + 40\sigma_3^2 - 15\sigma_2^3 \tag{3.10}$$

$$7! p_7 = 720\sigma_7 - 504\sigma_5\sigma_2 - 420\sigma_4\sigma_3 + 210\sigma_3\sigma_2^2 \tag{3.11}$$

$$\begin{aligned} 8! p_8 = &-5040\sigma_8 + 3360\sigma_6\sigma_2 + 2688\sigma_5\sigma_3 + 1260\sigma_4^2 \\ &- 1260\sigma_4\sigma_2^2 - 1120\sigma_3^2\sigma_2 + 105\sigma_2^4 \end{aligned} \tag{3.12}$$

$$9!p_9 = 40\,320\sigma_9 - 25\,920\sigma_7\sigma_2 - 20\,160\sigma_6\sigma_3 - 18\,144\sigma_5\sigma_4 + 9072\sigma_5\sigma_2^2 + 15\,120\sigma_4\sigma_3\sigma_2 + 2240\sigma_3^2 - 2520\sigma_3\sigma_2^3 \tag{3.13}$$

$$\begin{aligned} 10!p_{10} = {} & -362\,880\sigma_{10} + 226\,800\sigma_8\sigma_2 + 172\,800\sigma_7\sigma_3 \\ & + 151\,200\sigma_6\sigma_4 - 75\,600\sigma_6\sigma_2^2 + 72\,576\sigma_5^2 \\ & - 120\,960\sigma_5\sigma_3\sigma_2 - 56\,700\sigma_4^2\sigma_2 - 50\,400\sigma_4\sigma_3^2 \\ & + 18\,900\sigma_4\sigma_2^3 + 25\,200\sigma_3^2\sigma_2^2 - 945\sigma_2^5. \end{aligned} \tag{3.14}$$

It is not my intention to discuss detailed numerical computations, but an example hopefully suffices to illustrate the method. Consider the graph [6] for 3,4-dimethylenecyclobutene(I); its adjacency matrix is

$$\boldsymbol{A} = \begin{vmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{vmatrix} . \tag{3.15}$$

Upon calculating the traces of the powers of $\boldsymbol{A}$, we have:

$$\begin{array}{lll} \sigma_1 = 0, & \sigma_3 = 0, & \sigma_5 = 0 \\ \sigma_2 = 12, & \sigma_4 = 54, & \sigma_6 = 258. \end{array} \tag{3.16}$$

Newton's identities then yield

$$\begin{array}{lll} p_1 = 0, & p_3 = 0, & p_5 = 0 \\ p_2 = -6, & p_4 = 5, & p_6 = -1. \end{array} \tag{3.17}$$

Thus the characteristic polynomial is

$$P(G, \lambda) = \lambda^6 - 6\lambda^4 + 5\lambda^2 - 1. \tag{3.18}$$

This expression is the same as that obtained by Trinajstic [6] using Sach's theorem.

4. Comment

The technique employed by Balasubramanian [8] (and termed by him Frame's method) to construct the characteristic polynomial is nothing but symmetric functions and Newton's identities in disguise. In his method, the following matrices are constructed:

$$\begin{aligned} \boldsymbol{B}_1 &= \boldsymbol{A}^2 - p_1\boldsymbol{A} \\ \boldsymbol{B}_2 &= \boldsymbol{A}\boldsymbol{B}_1 + p_2\boldsymbol{A} \\ \boldsymbol{B}_3 &= \boldsymbol{A}\boldsymbol{B}_2 - p_3\boldsymbol{A} \\ \boldsymbol{B}_4 &= \boldsymbol{A}\boldsymbol{B}_3 + p_4\boldsymbol{A} \\ &\text{---------}. \end{aligned} \tag{4.1}$$

It can be shown that the characteristic polynomial coefficients p_n are given by

$$p_n = \frac{1}{n} \operatorname{tr} \boldsymbol{B}_{n-1}. \tag{4.2}$$

The right-hand side can be expressed in terms of σ_l and is simply Newton's identity. To see this consider, for example p_5. Repeated substitution of $\boldsymbol{B}_1$, $\boldsymbol{B}_2$ and $\boldsymbol{B}_3$ into $\boldsymbol{B}_4$ yields (upon assuming that $p_1 = 0$)

$$\boldsymbol{B}_4 = \boldsymbol{A}^5 + p_2\boldsymbol{A}^3 - p_3\boldsymbol{A}^2 + p_4\boldsymbol{A}. \tag{4.3}$$

Upon taking the trace of both sides and using Eq. (4.2), we have

$$p_5 = \tfrac{1}{5}(\sigma_5 + p_2\sigma_3 - p_3\sigma_2). \tag{4.4}$$

However, this is Newton's identity with $n = 5$, see Eq. (3.5).

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