On Evaluating the Characteristic Polynomial through Symmetric Functions

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We show how a unified approach through Newton's identities gives the coefficients of the characteristic polynomials in terms of symmetric powers of roots and vice-versa. We also provide some historical and modern references to the problem under consideration.

INTRODUCTION

The evaluation of the characteristic polynomial of a graph $\mathrm{Ch}(x) = \det(\mathbf{I}x - \mathbf{A})$ where $\mathbf{A}$ is the adjacency matrix of the graph, and $\mathbf{I}$, the identity matrix of the same size as $\mathbf{A}$, has been considered in chemical literature because of the invariants it provides for chemical structures in organic chemistry and because of the correlations that may exist between chemical properties and these invariants. (See Randić,[1] Barakat,[2] and references therein. A more modern reference that has a substantial bibliography is Zhang and Balasubramanian.[3]) In the second reference, Barakat presents a procedure for constructing the characteristic polynomial through the connection between the traces of powers of the adjacency matrix and the coefficients of the characteristic polynomial via Newton's identities. The method suggested by Barakat is to compute the powers of adjacency matrix and compute their traces, thereby getting the power sums of eigenvalues, and work recursively through Newton's identities to obtain elementary symmetric functions of the eigenvalues which are coefficients of the characteristic polynomial. Randić[1] observes that in the formulas

$$s_1 = -p_1$$

$$s_2 = p_1^2 - 2p_2$$

$$s_3 = -p_1^3 + 3p_1p_2 - 3p_3$$

$$s_4 = p_1^4 - 4p_1^2p_2 + 4p_1p_3 + 2p_2^2 - 4p_4 \tag{1}$$

$$s_5 = -p_1^5 + 5p_1^3p_2 - 5p_1^2p_3 - 5(p_2^2 - p_4)p_1 + 5(p_2p_3 - p_5)$$

$$\ldots$$

which solve for s_i's in terms of p_i's and in the formulas

$$1!p_1 = -s_1$$

$$2!p_2 = s_1^2 - s_2$$

$$3!p_3 = -s_1^3 + 3s_1s_2 - 2s_3$$

$$4!p_4 = s_1^4 - 6s_1^2s_2 + 3s_2^2 + 8s_1s_3 - 6s_4 \tag{2}$$

$$5!p_5 = -s_1^5 + 10s_1^3s_2 - 15s_1s_2^2 - 20s_1^2s_3 + 20s_2s_3 + 30s_1s_4 - 24s_5$$

$$\ldots$$

which do the reverse, the very simple pattern of Newton's identities seems to be lost and provides a combinatorial interpretation for the coefficients of (2) and illustrates it for the coefficients in the formula for p_{10} in terms of s_i's. This should be of interest because with this interpretation of coefficients, elementary functions for large matrices can be computed without the need for computing the smaller ones as required in a recursive method. In this note we give a method that proves *both* sets of formulas and interpret the coefficients of *both* sets of formulas combinatorially. We also provide some historical and current references to these formulas which go back to Waring, in the 18th century.

Remarks. We have presented the formulas in Randić[1] with some typographical corrections. We have also changed some signs to make the two sets of formulas (1) and (2) consistent. Also, formulas (2) are presented with $s_1 = 0$ there, since in the special case of the adjacency matrix of a graph, $s_1 = 0$ because the diagonal entries of the adjacency matrix are 0. This simplifies computations when the recursive approach through Newton's identities are used, but the combinatorial interpretation holds for the more general case. To get the formulas in Randić[1] and Barakat[2] all we need to do is set $s_1 = 0$ in our formulas. It should also be remarked that nowadays special cases of these formulas can be computed quite readily from Newton's identities using symbolic manipulation packages like Mathematica.

SOME NOTATION

If $\mathbf{A}$ is any $n \times n$ matrix, its characteristic polynomial is $\det(x\mathbf{I} - \mathbf{A})$. It factors into

$$\prod_{i=1}^{n}(x - \lambda_i)$$

where λ_i are the eigenvalues of the matrix. The coefficients $p_1, p_2, \ldots, p_n$ of the characteristic polynomial $x^n + p_1x^{n-1} + p_2x^{n-2} + \ldots + p_n$ are given in terms of the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ by $p_k = (-1)^k \sum \lambda_{i_1}\lambda_{i_2}\ldots\lambda_{i_k}$. The symmetric powers of the eigenvalues λ_i are defined by $s_k = \sum \lambda_i^k = \mathrm{Tr}(A^k)$. The summation here is over all the eigenvalues of $\mathbf{A}$.

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DERIVATION OF THE FORMULA FOR S_N'S IN TERMS OF P_N'S

As in Randić[1], we start with Newton's identities.

$$s_1 + p_1 = 0$$

$$s_2 + p_1 s_1 + 2p_2 = 0$$

$$s_3 + p_1 s_2 + p_2 s_1 + 3p_3 = 0$$

$$s_4 + p_1 s_3 + p_2 s_2 + p_3 s_1 + 4p_4 = 0$$

$$\ldots$$

Consider the formal power series $f(x) = \sum_{i=0}^{\infty} s_i x^i$ and $g(x) = \sum_{i=0}^{\infty} p_i x^i$. It is convenient to take $s_0 = 0$ and $p_0 = 1$. Then, Newton's identities are equivalent to the formal differential equation

$$f(x)g(x) + xg'(x) = 0$$

This can be solved by separating the variables:

$$\frac{f(x)}{x} = -\frac{g'(x)}{g(x)}$$

and

$$\int \frac{f(x)}{x} dx = -\int \frac{dg(x)}{g(x)} = -\ln g(x) + C$$

We can integrate the left side term by term to get

$$\int \sum_{i=1}^{\infty} s_i x^{i-1}\, dx = \sum_{i=1}^{\infty} s_i \frac{x^i}{i} = -\ln g(x) + C$$

When $x = 0$, the left side is 0 and the right side is C. So, C = 0 and we have two power series whose coefficients involve s_i and p_i, respectively:

$$\sum_{i=1}^{\infty} s_i \frac{x^i}{i} = -\ln g(x) = -\ln(1 + (g(x) - 1)) =$$

$$\sum_{i=1}^{\infty} (-1)^i \frac{(g(x) - 1)^i}{i} = \sum_{i=1}^{\infty} \frac{(-1)^i}{i} \left(\sum_{j=1}^{\infty} p_j x^j\right)^i$$

Expanding each inner infinite sum we get

$$-\sum_{n=1}^{\infty} p_n x^n + \frac{1}{2} \sum_{n=1}^{\infty} \Big(\sum_{\substack{i+j=n \\ i,j\geq 1}} p_i p_j \Big) x^n - \frac{1}{3} \sum_{n=1}^{\infty} \Big(\sum_{\substack{i+j+k=n \\ i,j,k\geq 1}} p_i p_j p_k \Big) x^n + \ldots$$

Therefore,

$$\frac{s_n}{n} = -p_n + \frac{1}{2} \sum_{\substack{i+j=n \\ i,j\geq 1}} p_i p_j - \frac{1}{3} \sum_{\substack{i+j+k=n \\ i,j,k\geq 1}} p_i p_j p_k + \ldots = \sum_{\substack{i_1+i_2+\ldots+i_n = k \\ i_1+2i_2+3i_3+\ldots+ni_n=n}} \frac{(-1)^k}{k} \frac{k!}{i_1! i_2! \ldots i_n!} p_1^{i_1} p_2^{i_2} \ldots p_n^{i_n}$$

where i_1, i_2, ..., i_n are non-negative integers. The last sum follows from the previous one by observing that terms with k p_i's appear in the summation with a coefficient of $(-1)^k/k$ and that there are $k!/(i_1!i_2!\ldots i_n!)$ of them if we specify that there are i_1 p_1's, i_2 p_2's, and so on. The numbers $k!/(i_1!i_2!\ldots i_n!)$ are coefficients that appear in the multinomial theorem and have the following combinatorial interpretation: They are the number of ways in which k mutually distinguishable balls can be put in n mutually distinguishable boxes so that the jth box contains i_j balls. This provides a combinatorial interpretation of the coefficients of the formulas for s_n's in terms of p_n's similar to the combinatorial interpretation given in Randić[1] for the coefficients of the formulas for p_n's in terms of s_n's.

Remark. While our approach to power series and the differential equation has been formal without considerations of convergence, the operations can be justified, for example, along the lines of Niven[4] or Henrici.[5]

THE FORMULA FOR P_N'S IN TERMS OF S_N'S

The same method gives the formulas (1) for p_n in terms of s_n also: Since $\ln (g(x)) = -\sum_{i=1}^{\infty} s_i x^i / i$, $g(x) = \exp(-\sum_{i=0}^{\infty} s_i x^i / i)$. Expanding using the power series for the exponential function,

$$g(x) = 1 - \frac{1}{1!} \sum_{i=1}^{\infty} s_i \frac{x^i}{i} + \frac{1}{2!} \left(\sum_{i=1}^{\infty} s_i \frac{x^i}{i} \right)^2 - \frac{1}{3!} \left(\sum_{i=1}^{\infty} s_i \frac{x^i}{i} \right)^3 + \ldots$$

Therefore, collecting coefficients of x^n in this series as before,

$$p_n = -\frac{1}{1!} \frac{s_n}{n} + \frac{1}{2!} \sum_{\substack{i+j=n \\ i,j\geq 1}} \frac{s_i s_j}{i\, j} - \frac{1}{3!} \sum_{\substack{i+j+k=n \\ i,j,k\geq 1}} \frac{s_i s_j s_k}{i\, j\, k} + \ldots = \sum_{\substack{i_1+i_2+\ldots+i_n=k \\ i_1+2i_2+3i_3+\ldots+ni_n=n}} \frac{(-1)^k}{k!} \frac{k!}{i_1! i_2! \ldots i_n!} \frac{s_1^{i_1} s_2^{i_2}}{1^{i_1}\, 2^{i_2}} \ldots \frac{s_n^{i_n}}{n^{i_n}} =$$

$$\sum_{\substack{i_1+i_2+\ldots+i_n=k \\ i_1+2i_2+3i_3+\ldots+ni_n=n}} \frac{(-1)^k}{i_1! i_2! \ldots i_n!} \frac{s_1^{i_1} s_2^{i_2}}{1^{i_1}\, 2^{i_2}} \ldots \frac{s_n^{i_n}}{n^{i_n}}$$

After we multiply both sides by $n!$, we get the formulas described in Randić[1] and in fact the magnitude of the coefficient $n!/1^{i_1} i_1! 2^{i_2} i_2! \ldots n^{i_n} i_n!$ is the number of permutations of n symbols composed of i_j cycles of length j for $j = 1,2, \ldots n$. See Abramovitz and Stegun.[6] This reference has the coefficients listed for the first ten formulas. It also provides a check on computations, viz.,

$$\sum_{\substack{i_1+i_2+\ldots+i_n=k \\ i_1+2i_2+3i_3+\ldots+ni_n=n}} \frac{n!}{1^{i_1} i_1! 2^{i_2} i_2! \ldots n^{i_n} i_n!}$$

equals $(-1)^{n-k}S_n^{(k)}$ where $S_n^{(k)}$ are the well-known Sterling numbers of the first kind.

HISTORICAL REMARKS

The formulas (1) and (2) are quite old. They are found, for example, in Burnside and Panton,[7] where they are derived by a somewhat different method and attributed to Waring who lived in the 18th century. A more modern reference is Knuth[8] which takes a slightly different generating function approach to the problem.

REFERENCES AND NOTES

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