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NOTE

ON THE EVALUATION OF THE CHARACTERISTIC POLYNOMIAL VIA SYMMETRIC FUNCTION THEORY

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Abstract

The use of power sum symmetric functions leads to Newton's identities, which relate the traces of various powers of A, the adjacency matrix of a graph, and the coefficients of the characteristic polynomials. While it is possible to solve Newton's identities and generate the coefficients by recursion or, alternatively, to derive them by sequential manipulations (yielding the explicit formulas), we show how the results can be expressed using a combinatorial approach and relate the evaluation of the coefficients to selected Young diagrams.

1. Introduction

The characteristic polynomial of a graph, $\mathrm{Ch}(x) = \det(A - Ix)$, where A is the adjacency matrix of the graph and I is the identity matrix of the same dimension, is one of the basic graph invariants. The characteristic polynomial, as well as spectral moments, has an important property: the coefficients are integers, and can be related to the enumeration of selected graph invariants. Interest in the characteristic polynomial also stems from the fact that it may reveal some relationship between the structure and the mathematical representation of the graph that can become obscured in non-integer data, such as eigenvalues. Several schemes for obtaining the characteristic polynomial have been discussed in the literature [1] and, in particular, it has been suggested that approaches based on the evaluation of traces of powers of the adjacency matrix are the most computationally simple [2]. In comparison, combinatorial approaches based on the enumeration of selected subgraphs, the first contribution

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to which appears to have been made by Coulson [3] but subsequently completely developed independently by several investigators [4], generally involve consideration of a large number of small subgraphs. Sachs formulated most completely the approach by showing that one need only consider subgraphs K_2 (isolated edges) and C_n (isolated cycles), and various combinations of these. The difficulty is that the number of components proliferates very quickly, and for graphs having a dozen or more vertices, the procedure may already be too cumbersome. An alternative is to start with the A matrix and its powers, either indirectly as in the so-called Krylov method [5] and the Frobenius method [6], or in the more direct approach described by Frame [7], to which Balasubramanian drew attention [2]. The method has already been used by the French atronomer Leverrier in the 1980s, as pointed out by Trinajstić and co-workers [8]. This approach can be related to Newton's identities, as recently pointed out by Barakat [9]. It appears that this scheme based on the use of traces of matrices has computational advantages, as discussed convincingly by Balasubramanian [2] and Barakat [9]. In particular, Balasubramanian developed a computer program that gives the coefficients of the characteristic polynomial for sizable graphs having over fifty vertices and some twenty cycles.

2. Outline of the symmetric function approach

The basis for the method was known even to Newton [10], who was involved in solving the equations associated with the characteristic polynomial. Symmetric functions of the roots of an equation are those functions in which all the roots are equally involved, so that the expression is unaltered in value when any two of the roots are interchanged [11]. The equations Newton considered can be written as [12]:

$$\begin{aligned} &s_1 + p_1 = 0 \\ &s_2 + p_1 s_1 + 2p_2 = 0 \\ &s_3 + p_1 s_2 + p_2 s_1 + 3p_3 = 0 \\ &s_4 + p_1 s_3 + p_2 s_2 + p_3 s_1 + 4p_4 = 0 \\ &\ldots\ldots \end{aligned} \tag{1}$$

Here, the p_k are the coefficients of the characteristic polynomial

$$\mathrm{Ch}(x) = x^n + p_1 x^{n-1} + p_2 x^{n-2} + \ldots + p_n ,$$

and the s_k are the traces of A^k [13]. The above equations need to be solved for all the s_k, and Burnside [12] gives the solution for the first initial s_k:

$$
\begin{aligned}
s_1 &= -p_1 \\
s_2 &= p_1^2 - 2p_2 \\
s_3 &= -p_1^3 + 3p_1p_2 - 3p_3 \\
s_4 &= p_1^4 - 4p_1^2p_2 + 4p_1p_2 + 2p_2^2 - p_4 \\
s_5 &= -p_1^5 + 5p_1^3p_2 - 5p_1^2p_3 - 5(p_2 - p_4)p_1 + 5(p_2p_3 - p_5) \\
&\ldots\ldots .
\end{aligned}
\tag{2}
$$

Observe that the very simply *pattern* of Newton's equations (1) – which allows one to write any line immediately from the previous one – has been lost in solving the equations, and any pattern in eqs. (2), the solutions for the s_k appear, at best, complicated. Barakat [9] considers the solutions for the p_k in terms of the s_k, obtaining the following explicit forms:

$$
\begin{aligned}
2!p_2 &= -s_2 \\
3!p_3 &= 2s_3 \\
4!p_4 &= -6s_4 + 3s_2^2 \\
5!p_5 &= 24s_5 - 20s_3s_2 \\
6!p_6 &= -120s_6 + 90s_4s_2 + 40s_3^2 - 15s_2^3 \\
&\ldots\ldots . \\
9!p_9 &= 40320s_9 - 25920s_7s_2 - 20160s_6s_3 - 18144s_5s_4 + 9072s_5s_2^2 \\
&\quad + 15120s_4s_3s_2 + 2240s_3^2 - 2520s_3s_2^3 \\
10!p_{10} &= -362880s_{10} + 226800s_8s_2 + 172800s_7s_3 + 15100s_6s_4 \\
&\quad - 75600s_6s_2^2 + 72576s_5^2 - 120960s_5s_3s_2 - 56700s_4^2s_2 \\
&\quad - 50400s_4s_3^2 + 18900s_4s_2^3 + 25200s_3^2s_2^2 - 945s_2^5 .
\end{aligned}
\tag{3}
$$

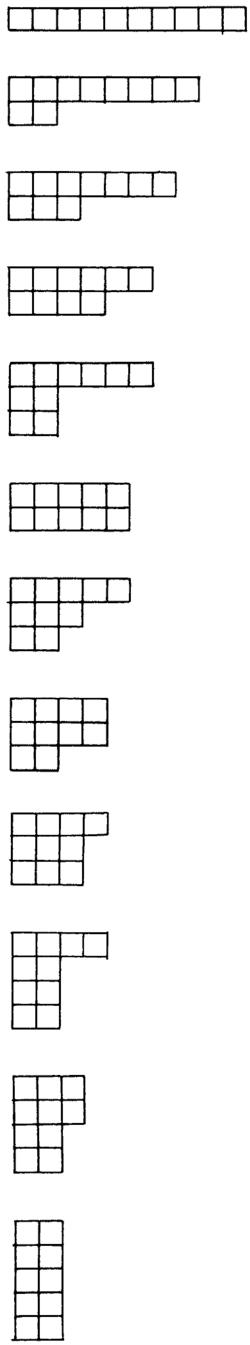
Again, any pattern to the solutions appears lost. It is disappointing that very simple expressions involving both s_k and p_k, when solved for either the s_k or p_k, appear to no longer show the simplicity that the original equations possess. However, as we will show, the above solutions for the p_k do have a relatively simple form if one recognizes the structural ingredients that are involved.

3. Structure of the coefficients

Let us first consider the terms appearing in the solution for p_k, which can be illustrated by considering p_{10}. The following terms appear:

$$s_{10},\ s_8 s_2,\ s_7 s_3,\ s_6 s_4,\ s_6 s_2^2,\ s_5^2,\ s_5 s_3 s_2,\ s_4^2 s_2,\ s_4 s_3^2,\ s_4 s_2^3,\ s_3^2 s_2^2,\ s_2^5 .$$

It is not difficult to recognize the above terms as various partitionings of 10, i.e. 10 + 0, 8 + 2, 7 + 3, 6 + 4, 6 + 2 + 2, 5 + 5, 5 + 3 + 2, 4 + 4 + 2, 4 + 3 + 3, 4 + 2 + 2 + 2, 3 + 3 + 2 + 2, and 2 + 2 + 2 + 2 + 2. The above are in fact all the possible partitionings of 10, excluding those involving 1. In fig. 1, we depict the above partitionings using Young diagrams [14]. The numerical values for the coefficients have also been included in fig. 1. The question now is to consider whether there is some relationship between the particular diagram and the magnitudes of the corresponding coefficients. It is easy to see that the signs of the coefficients alternate just as the number of rows in the Young diagram increases: the odd number of rows for p_{10} gives a negative sign (the opposite is the case with p_9, as illustrated in fig. 2). The only other apparent and helpful observation is the fact that the magnitudes decrease as the number of rows increases, or if the rows have less dissimilar "lengths". This suggests that such terms have fewer and fewer factors. Because the leading coefficient can be recoginized as 10!/10, this suggests that we may have a simple recipe for deriving other coefficients by dividing 10! by suitable other numbers. One immediately finds that 10!/8 · 2 = 226800; hence, the numbers 8 and 2, which characterize the partitioning of 10, also indicate the factors. It is now easy to verify that this is indeed the rule for obtaining the other coefficients, *if* no two rows have the same number of elements (boxes). In the case of the partition 5 + 5, instead of 72576 we obtain twice this value. Likewise, for the partition 4 + 4 + 2, we obtain 10!/4 · 4 · 2 = 113400 instead of 56700. In the case that a single term in the partition repeats itself three times (e.g. 4 + 2 + 2 + 2), we obtain a number six times too large, which suggests an additional factor of 3! Indeed, as one can verify for the partitions 3 + 3 + 2 + 2 and 2 + 2 + 2 + 2 + 2, when identical terms appear in the partition we have to divide by the corresponding factorial, resulting in 10!/(3 · 3 · 2 · 2) (2!) (2!) and 10!/(2 · 2 · 2 · 2 · 2) (5!), respectively. We can thus formulate simple rules for the magnitudes of the coefficients of various characteristic polynomials:



$362880 = 10!/10$

$226800 = 10!/8 \cdot 2$

$172800 = 10!/7 \cdot 3$

$151200 = 10!/6 \cdot 4$

$75600 = 10!/6 \cdot 2 \cdot 2 \cdot 2!$

$72576 = 10!/5 \cdot 5 \cdot 2!$

$120960 = 10!/5 \cdot 3 \cdot 2$

$56700 = 10!/4 \cdot 4 \cdot 2 \cdot 2!$

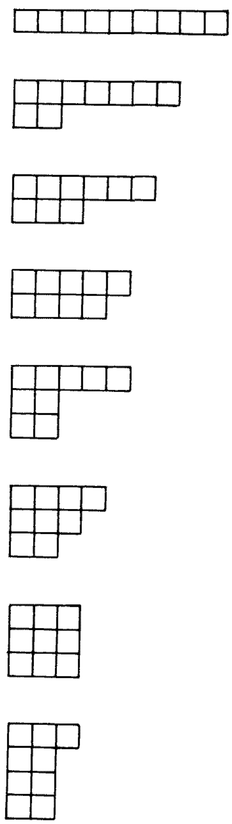
$50400 = 10!/4 \cdot 3 \cdot 3 \cdot 2!$

$18900 = 10!/4 \cdot 2 \cdot 2 \cdot 2 \cdot 3!$

$25200 = 10!/3 \cdot 3 \cdot 2 \cdot 2 \cdot 2! \cdot 2!$

$945 = 10!/2^5 \cdot 5!$

Fig. 1. Young diagrams and the associated coefficients of $10!p_{10}$ decomposed into factors governed by the form of the diagrams.



$40320 = 9!/9$

$25920 = 9!/7 \cdot 2$

$20160 = 9!/6 \cdot 3$

$18144 = 9!/5 \cdot 4$

$9072 = 9!/5 \cdot 2^2 \cdot 2!$

$15120 = 9!/4 \cdot 3 \cdot 2$

$2240 = 9!/3^3 \cdot 3!$

$2520 = 9!/3 \cdot 2^3 \cdot 3!$

Fig. 2. Young diagrams and the decomposition of the coefficients of $9!p_9$.

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$n!p_n$ is given by the sum of the terms derived from all possible partitionings of n, excluding terms involving 1 as a component. Signs are determined by the product of the parities of R and C, where R, C represent the number of rows and columns in the associated Young diagrams. The magnitude of the term is determined by the quotient $k!/\Sigma m^n n!$, where m is summed over all partitionings of k (excluding those involving 1), and n gives the multiplicity (degeneracy) of the corresponding m.

With the above rule, one can write down the set of equations giving explicit values for the p_k by inspection, achieving again the simplicity of the original equations of Newton.

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