Note on Algebraic Structure Count

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Three recursion relations for the algebraic structure count are deduced, which are closely analogous to the well-known recursion relation for the number of Kekulé structures. An efficient graphical method for the calculation of algebraic structure count is proposed.

It is a long known result [1] that the determinant of the adjacency matrix (A) of a benzenoid graph is related to the number of the Kekulé structures (K) of the corresponding molecule as

\[ \det A = (-1)^{n/2} K^2. \]  

(1)

For non-benzenoid (but alternant) systems, (1) is no more applicable and has to be replaced by

\[ \det A = (-1)^{n/2} L^2 \]  

with \( L \) being a certain integer [2].

In the above equations and later on, \( n \) denotes the number of vertices of the molecular graph. It may be assumed that \( n \) is even since otherwise \( K = L = 0 \).

The quantity \( L \) has been called [3, 4] the “algebraic structure count” (or “corrected structure count” [5, 6]). Its relation to the Kekulé structures has been extensively examined [6–8]. The algebraic structure count plays an important role in the topological theory of non-benzenoid conjugated molecules [6, 9–12].

Let \( e \) be an (arbitrary) edge of the molecular graph \( G \). Then \( G - e \) will denote the subgraph obtained by deleting this edge from \( G \). In addition, \( G - (e) \) will denote the subgraph obtained from \( G \) by deletion of the two vertices which are incident to \( G \). Hence, if \( G \) has \( n \) vertices, then \( G - e \) and \( G - (e) \) have \( n \) and \( n - 2 \) vertices, respectively.

The number of Kekulé structures of a molecular graph can be easily calculated by means of the recursion formula [6]

\[ K(G) = K(G - e) + K(G - (e)). \]  

(3)

On the other hand, no analogous regularity has been previously observed for the algebraic structure count. The aim of the present paper is to show that \( L(G) \), \( L(G - e) \) and \( L(G - (e)) \) conform to one of the following three relations:

\[ L(G) = L(G - e) + L(G - (e)), \]  

(4)

\[ L(G) = L(G - e) - L(G - (e)), \]  

(5)

\[ L(G) = L(G - (e)) - L(G - e) \]  

(6)

which, of course, closely resemble (3).

As a matter of fact, (4), (5) and (6) may apply in the case of alternant non-benzenoid systems. This is illustrated by the example of the molecular graph \( G_0 \), whose three edges are labelled by \( e_1, e_2 \) and \( e_3 \). The corresponding subgraphs \( G_0 - e_i \) and \( G_0 - (e_i) \), \( i = 1, 2, 3 \), are given as follows:

Direct calculation shows that \( L(G_0) = 4 \) (see later), whereas \( L(G_0 - e_1) = L(G_0 - (e_1)) = L(G_0 - e_2) = 2, L(G_0 - e_3) = 6, L(G_0 - e_3) = 0 \) and \( L(G_0 - (e_3)) = 4 \). Thus (4) holds in the case of the deletion of the edge \( e_1 \), (5) applies for the edge \( e_2 \), and (6) must be used if the edge \( e_3 \) is being deleted.

In order to deduce (4)–(6), recall that the characteristic polynomial \( \Phi(G) \) of the graph \( G \) is defined via

\[ \Phi(G) = \Phi(G, x) = \det (x I - A), \]  

(7)

where \( I \) is the unit matrix of dimension \( n \). Then, because of (2),

\[ \Phi(G, 0) = (-1)^{n/2} L^2. \]  

(8)
The characteristic polynomial conforms to the relations \[\Phi(G) = \Phi(G - e) - \Phi(G - (e)) - 2 \sum_Z \Phi(G - Z), \quad (9)\]
where the summation embraces all cycles \(Z\) which contain the edge \(e\), and \[\Phi(G - v_r) \Phi(G - v_s) - \Phi(G) \Phi(G - v_r - v_s)
= \left( \sum_W \Phi(G - W) \right)^2, \quad (10)\]
where \(v_r\) and \(v_s\) are two vertices of \(G\) and the r.h.s. summation goes over all paths \(W\) which connect the vertices \(v_r\) and \(v_s\). If \(v_r\) and \(v_s\) are adjacent vertices (joined by the edge \(e\)), then (10) can be rewritten in the form \[\Phi(G - v_r) \Phi(G - v_s) - \Phi(G) \Phi(G - (e))
= \left( \Phi(G - (e)) + \sum_Z \Phi(G - Z) \right)^2. \quad (11)\]
Setting \(x = 0\) into (9) and having (8) in mind, we get \[L(G)^2 = L(G - e)^2 + L(G - (e))^2 + 2S, \quad (12)\]
where \[S = \sum_Z (-1)^{(z_2-1)}/2 \Phi(G - Z)^2 \quad (13)\]
and \(z\) is the size of the cycles \(Z\). (Note that if \(Z\) is of size \(4m + 2\), then \((-1)^{(z_2-1)/2} = +1\), and if \(Z\) is of size \(4m\), then \((-1)^{(z_2-1)/2} = -1\). Cycles of odd size cannot occur in the molecular graphs of alternant systems.)

Set now \(x = 0\) into (11). Since \(n\) is even, the graphs \(G - v_r\) and \(G - v_s\) have an odd number of vertices and therefore \(\Phi(G - v_r, 0) = \Phi(G - v_s, 0) = 0\). Consequently, we get from (11) \[L(G)^2 L(G - (e))^2 = [L(G - (e))^2 + S]^2. \quad (14)\]
Eliminating the auxiliary quantity \(S\) from (12) and (14), we arrive at an identity connecting \(L(G)\), \(L(G - e)\) and \(L(G - (e))\): \[4L(G)^2 L(G - (e))^2 = \left[ L(G)^2 + L(G - (e))^2 - L(G - e)^2 \right]^2. \quad (15)\]

The above relation can be further transformed into \([L(G) - L(G - (e)) - L(G - e)]\) \[\cdot [L(G) - L(G - (e)) + L(G - e)]\] \[\cdot [L(G) + L(G - (e)) - L(G - e)]\] \[\cdot [L(G) + L(G - (e)) + L(G - e)] = 0. \quad (16)\]

Since the last factor on the left-hand side of (16) is evidently non-zero, we conclude that the condition (15) implies the validity of either (4) or (5) or (6).

A detailed analysis of the relation (15) shows that formula (5) holds if the term \(L(G - (e)) + S\) is negative (or zero). Formulas (4) and (6) hold when \(L(G - (e)) + S\) is positive (or zero). Presently we are not able to determine the conditions which would make possible to predict whether (4) or (6) will apply for a given edge \(e\) of a given graph \(G\).

In spite of their simple algebraic form, the recursion formulas (4)-(6) are of little value for the actual calculation of the algebraic structure count. For practical purposes, (12) provides a much more efficient method of calculation of the algebraic structure count.

The use of (12) will be illustrated by the example of the graph \(G_0\). The edge which will be deleted is \(e_3\). There are four cycles in \(G_0\) which contain \(e_3\). They will be labelled by \(Z_1, Z_2, Z_3\) and \(Z_4\). The corresponding cycle-deleted subgraphs are given as follows:

\[\begin{align*}
\text{\(Z_1\)} & \quad \text{\(G_0 - Z_1\)} \\
\text{\(Z_2\)} & \quad \text{\(G_0 - Z_2\)} \\
\text{\(Z_3\)} & \quad \text{\(G_0 - Z_3\)} \\
\text{\(Z_4\)} & \quad \text{\(G_0 - Z_4\)}
\end{align*}\]

We already know that \(L(G_0 - e_3) = 0\) and \(L(G_0 - (e_3)) = 4\). A simple calculation shows that in addition \(L(G_0 - Z_1) = L(G_0 - Z_2) = L(G_0 - Z_3) = L(G_0 - Z_4) = 2\). Since \(z_1 = 4, \ z_2 = 8, \ z_3 = 6\) and \(z_4 = 10\), we have \[L(G_0)^2 = 0^2 + 4^2 + 2(-2^2 - 2^2 + 2^2 + 2^2) = 16\]
and therefore \(L(G_0) = 4\).