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The Vertex Graphical Condensation for Algebraic Structure Count of Molecular Graphs

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Abstract

The algebraic structure count of a bipartite graph $G = (U, V)$, denoted by $L(G)$, is defined as the difference between the number of so-called "even" and "odd" Kekulé structures of G by Wilcox in theoretical organic chemistry. Let $e = uv$ be an edge of a bipartite graph G. Gutman proved that G satisfies one of the following relations:

$$L(G) = L(G - e) + L(G - u - v),$$
$$L(G) = L(G - e) - L(G - u - v),$$
$$L(G) = -L(G - e) + L(G - u - v),$$

where $G - e$ (resp. $G - u - v$) is the graph obtained from G by deleting edge e (resp. vertices u and v). In this short note, we obtain a similar result and prove that for any $u_1, u_2 \in U, v_1, v_2 \in V$, G satisfies one of the following relations:

$$L(G)L(G - u_1 - u_2 - v_1 - v_2) =$$
$$L(G - u_1 - v_1)L(G - u_2 - v_2) + L(G - u_1 - v_2)L(G - u_2 - v_1),$$
$$L(G)L(G - u_1 - u_2 - v_1 - v_2) =$$
$$L(G - u_1 - v_1)L(G - u_2 - v_2) - L(G - u_1 - v_2)L(G - u_2 - v_1),$$
$$L(G)L(G - u_1 - u_2 - v_1 - v_2) =$$
$$-L(G - u_1 - v_1)L(G - u_2 - v_2) + L(G - u_1 - v_2)L(G - u_2 - v_1).$$

1 Introduction

Let $G = (U, V)$ be a bipartite graph with bipartition $U \cup V$, if not specified. The algebraic structure count of G, denoted by $L(G)$, is defined as the square root of the absolute value of the determinant of the adjacency matrix $A(G)$ of G [11, 12, 15, 16], that is,

$$L(G) = \sqrt{|\det(A(G))|}. \quad (1)$$

Let $|U| = m, |V| = n$. It is well known that $L(G)^2 = (-1)^n \det(A(G))$ if $m = n$ and $L(G) = 0$ otherwise [8]. Hence we may assume that $G = (U, V)$ is a bipartite graph with $|U| = |V| = n$. If G is a benzenoid graph, then

$$K(G)^2 = (-1)^n \det(A(G)), \tag{2}$$

where $K(G)$ is the number of perfect matchings (Kekulé structures) of G [5]. Hence if G is a benzenoid graph, then

$$L(G) = K(G). \tag{3}$$

The algebraic structure count of a bipartite graph is related closely the thermodynamic stability of the corresponding alternant hydrocarbons. It has important applications in theoretical organic chemistry [7, 10, 11, 14, 17]. In particular, if $L(G) = 0$, then the respective hydrocarbon is extremely reactive and usually does not exist [10, 17]. See for example some related references [1–4, 9, 13] on the algebraic structure count.

Note that for any edge $e = uv$ in a graph G, $K(G)$ satisfies the following recurrence relation

$$K(G) = K(G - e) + K(G - u - v), \tag{4}$$

where $G - e$ (resp., $G - u - v$) is the graph obtained from G by deleting edge e (resp., vertices u and v). Motivated by this result, Gutman [9] proved that $L(G), L(G - e)$ and $L(G - u - v)$ conform to one of the following three relations:

$$L(G) = L(G - e) + L(G - u - v), \tag{5}$$

$$L(G) = L(G - e) - L(G - u - v), \tag{6}$$

$$L(G) = -L(G - e) + L(G - u - v), \tag{7}$$

In linear algebra, the well-known Dodgson's determinant-evaluation rule [6] implies that, for any square matrix $M = (m_{ij})_{n\times n}$ of order n,

$$\det(M)\det(M_{1n}^{1n}) = \det(M_1^1)\det(M_n^n) - \det(M_1^n)\det(M_n^1), \tag{8}$$

where M_{1n}^{1n} (resp., M_i^j) is the matrix obtained from M be deleting two rows and two columns 1 and n (resp., the ith row and jth column).

Motivated by Eqs. (5)-(8), in this note, we obtain a similar result to Eqs. (5)-(7) and prove that for any $u_1, u_2 \in U, v_1, v_2 \in V$ in a bipartite graph $G = (U, V)$, G satisfies the one of the following relations:

$$L(G)L(G-u_1-u_2-v_1-v_2) = L(G-u_1-v_1)L(G-u_2-v_2)+L(G-u_1-v_2)L(G-u_2-v_1), \tag{9}$$

$$L(G)L(G-u_1-u_2-v_1-v_2) = L(G-u_1-v_1)L(G-u_2-v_2)-L(G-u_1-v_2)L(G-u_2-v_1), \tag{10}$$

$$L(G)L(G-u_1-u_2-v_1-v_2) = -L(G-u_1-v_1)L(G-u_2-v_2)+L(G-u_1-v_2)L(G-u_2-v_1). \tag{11}$$

2 Proof of the main result

Note that $G = (U, V)$ is a bipartite graph. If $|U| \neq |V|$, then $L(G) = L(G - u_1 - u_2 - v_1 - v_2) = L(G - u_1 - v_1) = L(G - u_2 - v_2) = L(G - u_1 - v_2) = L(G - u_2 - v_1) = 0$. Hence we can assume that $|U| = |V| = n$. Let $U = \{u'_1, u'_2, \ldots, u'_n\}, V = \{v'_1, v'_2, \ldots, v'_n\}$. The bipartite adjacency matrix of G, denoted $B(G) = (b_{ij})_{n\times n}$, is defined as follows:

$$b_{ij} = \begin{cases} 1 & \text{if } u'_i v'_j \text{ is an edge of } G, \\ 0 & \text{otherwise.} \end{cases}$$

Obviously, the adjacency matrix of G can be expressed by

$$A(G) = \begin{pmatrix} 0 & B(G) \\ B(G)^T & 0 \end{pmatrix},$$

where $B(G)^T$ is the transpose of $B(G)$. Hence

$$\det(A(G)) = (-1)^n \det(B(G))^2. \tag{12}$$

By Eqs. (1) and (12),

$$L(G) = |\det(B(G))|. \tag{13}$$

Without loss of generality, set $u'_1 = u_1, u'_n = u_2, v'_1 = v_1, v'_n = v_2$. Using Dodgson's determinant-evaluation rule Eq. (8) to $B(G)$, then

$$det(B(G)) \det(B(G)^{1n}_{1n}) = \det(B(G)^1_1) \det(B(G)^n_n) - \det(B(G)^n_1) \det(B(G)^1_n). \tag{14}$$

where $B(G)^{1n}_{1n}$ (resp., $B(G)^j_i$) is the matrix obtained from $B(G)$ be deleting two rows and two columns 1 and n (resp., the ith row and jth column). By the definition of the bipartite adjacency matrix of a bipartite graph, it is not difficult to see that $B(G)^{1n}_{1n}$ (resp.,

$B(G)_1^1, B(G)_n^n, B(G)_1^n, B(G)_n^1)$ is the bipartite adjacency matrix of $G - u_1 - u_2 - v_1 - v_2$ (resp., $G - u_1 - v_1, G - u_2 - v_2, G - u_1 - v_2, G - u_2 - v_1$). Hence, by Eq. (13),

$$L(G - u_1 - u_2 - v_1 - v_2) = |\det(B(G)_{1n}^{1n})|, \tag{15}$$

$$L(G - u_1 - v_1) = |\det(B(G)_1^1)|, \tag{16}$$

$$L(G - u_2 - v_2) = |\det(B(G)_n^n)|, \tag{17}$$

$$L(G - u_1 - v_2) = |\det(B(G)_1^n)|, \tag{18}$$

$$L(G - u_2 - v_1) = |\det(B(G)_n^1)|, \tag{19}$$

Note that $L(G)L(G - u_1 - u_2 - v_1 - v_2) \geq 0$. Then Eqs. (9), (10) and (11) are immediate from Eqs. (13)-(19).

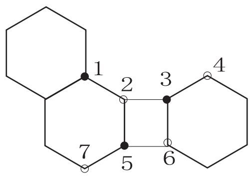

Figure 1. A molecular graph G.

3 Discussion

For the molecular graph G illustrated in Figure 1, it is not difficult to show that it satisfies: $L(G) = 4, L(G-1-2-3-4) = 1, L(G-2-3-5-6) = 2, L(G-1-2-5-7) = 2; L(G-1-2) = 2, L(G-3-4) = 3, L(G-1-4) = 1, L(G-2-3) = 2, L(G-5-6) = 2, L(G-2-5) = 4, L(G-3-6) = 3, L(G-5-7) = 2, L(G-1-7) = 1$. Hence

$$L(G)L(G-1-2-5-7) = L(G-1-2)L(G-5-7) + L(G-1-7)L(G-2-5),$$

$$L(G)L(G-1-2-3-4) = L(G-1-2)L(G-3-4) - L(G-1-4)L(G-2-3),$$

$$L(G)L(G-2-3-5-6) = -L(G-2-3)L(G-5-6) + L(G-2-5)L(G-3-6).$$

Thus, a natural question is: For any $u_1, u_2 \in U, v_1, v_2 \in V$ in a bipartite graph $G = (U, V)$, how to determine which equation among Eqs. (9)-(11) holds?

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References

[1] O. Bodroža–Pantić, Algebraic structure count of some cyclic hexagonal-square chains on the Möbius strip, *J. Math. Chem.* **41** (2007) 283–294.

[2] O. Bodroža–Pantić, S. J. Cyvin, I. Gutman, A formula for the algebraic structure count of multiple phenylenes, *MATCH Commun. Math. Comput. Chem.* **32** (1995) 47–58.

[3] O. Bodroža–Pantić, I. Gutman, S. J. Cyvin, Algebraic structure count of some non-benzenoid conjugated polymers, *ACH Models Chem.* **133** (1996) 27–41.

[4] O. Bodroža–Pantić, A. Ilic–Kovacevic, Algebraic structure count of angular hexagonal-square chains, *Fibonacci Quart.* **45** (2007) 3–9.

[5] M. J. S. Dewar and H. C. Longuet–Higgins, The correspondence between the resonance and molecular orbital theories, *Proc. Roy. Soc. (London) A* **214** (1952) 482–493.

[6] C. L. Dodgson, Condensation of determinants, *Proc. Roy. Soc. London* **15** (1866) 150–155.

[7] A. Graovac, I. Gutman, N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer–Verlag, Berlin, 1977.

[8] A. Graovac, I. Gutman, The determinant of the adjacency matrix of a molecular graph, *MATCH Commun. Math. Comput. Chem.* **6** (1979) 49–73.

[9] I. Gutman, Note on algebraic structure count, *Z. Naturforsch.* **39a** (1984) 794–796.

[10] I. Gutman, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbits, X. The number of Kekulé structures and the thermodynamic stability of conjugated systems, *Tetrahedron* **31** (1975) 143–146.

[11] W. C. Herndon, Resonance theory and the enumeration of Kekulé structures, *J. Chem. Edu.* **51** (1974) 10–15.

[12] W. C. Herndon, Enumeration of resonance structures, *Tetrahedron* **29** (1973) 3–12.

[13] D. J. Klein, T. G. Schmalz, S. EI–Basil, M. Randić, N. Trinajstić, Kekulé count and algebraic structure count for unbranched alternant cata–fusenes, *J. Mol. Struct. (Theochem)* **179** (1988) 99–107.

[14] C. F. Wilcox, A topological definition of resonance energy, *Croat. Chem. Acta* **47** (1975) 87–94.

[15] C. F. Wilcox, Stability of molecules containing $(4n)$-rings, *Tetrahedron Lett.* **9** (1968) 795–800.

[16] C. F. Wilcox, Stability of molecules containing nonalternant rings, *J. Am. Chem. Soc.* **91** (1969) 2732–2736.

[17] C. F. Wilcox, I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, XI. Aromatic substitution, *Tetradedron* **31** (1975) 147–152.