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New Variants of Gutman's Formulas on the Algebraic Structure Count

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Abstract

Let $C(G)$ denote the algebraic structure count of a bipartite graph G with bipartition (V_1, V_2). Gutman proved that, for any edge $e = ab$ of G, one of the following formulas holds:

$$C(G) = C(G-e) + C(G-a-b),$$
$$C(G) = C(G-e) - C(G-a-b),$$
$$C(G) = C(G-a-b) - C(G-e).$$

In this paper, we prove that, for any pair of independent edges $\{f = uv, g = wx\}$ of G, then one of the following formulas holds.

$$C(G)C(G-f-g) = C(G-f)C(G-g) + C(G-u-x)C(G-w-v),$$
$$C(G)C(G-f-g) = C(G-f)C(G-g) - C(G-u-x)C(G-w-v),$$
$$C(G)C(G-f-g) = C(G-u-x)C(G-w-v) - C(G-f)C(G-g),$$

where $u, w \in V_1, v, x \in V_2$. We prove also that, for any edge $h = yz$ and two vertices r and s such that $y, r \in V_1$ and $z, s \in V_2$ and $\{y, z\} \cap \{r, s\} = \emptyset$, then one of the following formulas holds.

$$C(G)C(G-h-r-s) = C(G-h)C(G-r-s) + C(G-y-s)C(G-r-z),$$
$$C(G)C(G-h-r-s) = C(G-h)C(G-r-s) - C(G-y-s)C(G-r-z),$$
$$C(G)C(G-h-r-s) = C(G-y-s)C(G-r-z) - C(G-h)C(G-r-s).$$

1 Introduction

Suppose that G is a bipartite graph with bipartition (V_1, V_2). In theoretical organic chemistry, Wilcox [16, 17] defined the algebraic structure count of

G, denoted by $C(G)$, as the difference between the number of so-called "even" and "odd" perfect matchings of G. Let $A(G)$ be the adjacency matrix of G. It is well known [6,8] that the determinant of $A(G)$ satisfies:

$$\det(A(G)) = (-1)^{\frac{|V_1|+|V_2|}{2}} C(G)^2, \tag{1}$$

and if each "nice" cycle C_l in G satisfies $l = 2$ $(mod\ 4)$, then

$$\det(A(G)) = (-1)^{\frac{|V_1|+|V_2|}{2}} M(G)^2, \tag{2}$$

if $|V_1| + |V_2|$ is even, and $\det(A(G)) = 0$ otherwise, where a cycle C_l is called to be "nice" if $G - C_l$ has perfect matchings (or Kekulé structures), and $M(G)$ is the number of perfect matchings of G. Hence if each "nice" cycle C_l in G satisfies $l = 2$ $(mod\ 4)$, then

$$C(G) = M(G), \tag{3}$$

i.e., the algebraic structure count of G equals the number of perfect matchings of G. The relation between $C(G)$ and $M(G)$ has been studied extensively [5, 10, 13]. On the other hand, $C(G)$ has a closed relation with the thermodynamic stability of the corresponding molecular graphs and has important applications in theoretical organic chemistry [9, 12, 13, 15, 18]. On the further research on $C(G)$, see references [1–4, 11, 14, 19].

It is well known that, for any edge $e = xy$ of G, the number of perfect matchings of G satisfies:

$$M(G) = M(G - x - y) + M(G - e), \tag{4}$$

where $G-x-y$ (or $G-e$) is the graph obtained from G by deleting vertices x and y (or e). Gutman [11] obtained a similar result to Eq. (4) for the algebraic structure count, and proved that one of the following relations holds.

$$C(G) = C(G - e) + C(G - x - y), \tag{5}$$

$$C(G) = C(G - e) - C(G - x - y), \tag{6}$$

$$C(G) = C(G - x - y) - C(G - e). \tag{7}$$

Motivated by Eqs. (5), (6) and (7), we obtained a variant of Gutman's formulas above as follows. Let G be a bipartite graph with bipartition (V_1, V_2). For any $a, c \in V_1, b, d \in V_2$, then one of the following relations holds.

$$C(G)C(G-a-b-c-d) = C(G-a-b)C(G-c-d)+C(G-a-d)C(G-b-c),$$

$$C(G)C(G-a-b-c-d) = C(G-a-b)C(G-c-d)-C(G-a-d)C(G-b-c),$$

$$C(G)C(G-a-b-c-d) = C(G-a-d)C(G-b-c)-C(G-a-b)C(G-c-d).$$

Further to the result above, in this paper, we continue to study the new variants of Gutman's formulas above and prove mainly the following theorems, whose proofs will be given in the next section.

Theorem 1.1. Let G be a bipartite graph with bipartition (V_1, V_2). For any pair of independent edges $\{f = uv, g = wx\}$ of G, then one of the following formulas holds.

$$C(G)C(G - f - g) = C(G - f)C(G - g) + C(G - u - x)C(G - w - v),$$
$$C(G)C(G - f - g) = C(G - f)C(G - g) - C(G - u - x)C(G - w - v),$$
$$C(G)C(G - f - g) = C(G - u - x)C(G - w - v) - C(G - f)C(G - g),$$

where $u, w \in V_1, v, x \in V_2$.

Theorem 1.2. Let G be a bipartite graph with bipartition (V_1, V_2). For any edge $h = yz$ and two vertices r and s such that $y, r \in V_1$ and $z, s \in V_2$ and $\{y, z\} \cap \{r, s\} = \emptyset$, then one of the following formulas holds.

$$C(G)C(G-h-r-s) = C(G-h)C(G-r-s)+C(G-y-s)C(G-r-z),$$
$$C(G)C(G-h-r-s) = C(G-h)C(G-r-s)-C(G-y-s)C(G-r-z),$$
$$C(G)C(G-h-r-s) = C(G-y-s)C(G-r-z)-C(G-h)C(G-r-s).$$

2 Proofs of main results

Let M be a matrix of order n. We use $M_{i_1 i_2 \ldots i_k}^{j_1 j_2 \ldots j_k}$ to denote the matrix obtained from M by deleting k rows $i_1, i_2, \ldots, i_k$ and k columns $j_1, j_2, \ldots, j_k$. We need to introduce some lemmas as follows.

Lemma 2.1. (Dodgson, [7]) Let $P = (p_{ij})$ be a real matrix of order $n \geq 3$. Then

$$\det(P)\det(P_{1n}^{1n}) = \det(P_1^1)\det(P_n^n) - \det(P_1^n)\det(P_n^1). \tag{8}$$

Now, we use the Dodgson's determinant-evaluation rule above to prove the following lemmas which will play a key role in the proofs of the main results.

Lemma 2.2. Let $P = (p_{ij})$ be a real matrix of order $n \geq 3$ and $p_{nn} \neq 0$. Let $Q = (q_{ij})$ be the matrix obtained from P by replacing entry p_{nn} with 0, i.e., $q_{ij} = p_{ij}$ if $(i,j) \neq (n,n)$ and $q_{nn} = 0$. Then

$$\det(P)\det(Q_1^1) = \det(P_1^1)\det(Q) + p_{nn}\det(P_n^1)\det(P_1^n). \tag{9}$$

Proof. Let

$$X = \begin{pmatrix} Q & -\alpha_n^T \\ \alpha_n & 1 \end{pmatrix},$$

where $\alpha_n = (0, 0, \ldots, 0, c)$ is a vector with n entries, $c = \sqrt{p_{nn}}$ if $p_{nn} > 0$ and $c = i\sqrt{-p_{nn}}$ if $p_{nn} < 0, i^2 = -1$, and α_n^T is the transpose of α_n. Obviously, X is a matrix of order $n+1$. Using Lemma 2.1,

$$\det(X)\det\left(X_{1(n+1)}^{1(n+1)}\right) = \det(X_1^1)\det(X_{n+1}^{n+1}) - \det(X_1^{n+1})\det(X_{n+1}^1). \tag{10}$$

Note that

$$\det(X) = \det\begin{pmatrix} Q & -\alpha_n^T \\ \alpha_n & 1 \end{pmatrix}$$

$$= \det\begin{pmatrix} Q + \alpha_n^T\alpha_n & -\alpha_n^T \\ 0 & 1 \end{pmatrix} = \det\left(Q + \alpha_n^T\alpha_n\right).$$

By the definition of P, Q and X, it is not difficult to see that

$$Q + \alpha_n^T \alpha_n = P, \tag{11}$$

$$X_{1(n+1)}^{1(n+1)} = Q_1^1, X_{n+1}^{n+1} = Q. \tag{12}$$

Hence

$$\det(X) = \det(P). \tag{13}$$

Similarly,

$$\det(X_1^1) = \det \begin{pmatrix} Q_1^1 & -\beta_{n-1}^T \\ \beta_{n-1} & 1 \end{pmatrix} = \det\left(Q_1^1 + \beta_{n-1}^T \beta_{n-1}\right) = \det(P_1^1), \tag{14}$$

$$\det(X_1^{n+1}) = \det \begin{pmatrix} Q_1 \\ \alpha_n \end{pmatrix} = c\det(Q_1^n) = c\det(P_1^n), \tag{15}$$

$$\det(X_{n+1}^1) = \det\left(Q^1, -\alpha_n^T\right) = -c\det(Q_n^1) = -c\det(P_n^1). \tag{16}$$

where $\beta_{n-1} = (0, 0, \ldots, 0, c)$ is a vector with $n-1$ entries, Q_1 is the matrix obtained from Q by deleting the first row, and Q^1 is the matrix obtained from Q by deleting the first column.

By Eqs. (10) and (12)-(16), Eq. (9) is immediate. Hence the lemma follows. ∎

Let $M = (m_{ij})$ be a real matrix of order $n \geq 3$ and $m_{11}m_{nn} \neq 0$. Define three matrices $R = (r_{ij}), S = (s_{ij})$ and $T = (t_{ij})$ of order n from M such that

$$r_{ij} = \begin{cases} m_{ij}, \text{ if } (i,j) \neq (1,1), (n,n) \\ 0, \text{ if } (i,j) = (1,1), (n,n) \end{cases},$$

$$s_{ij} = \begin{cases} m_{ij}, \text{ if } (i,j) \neq (1,1) \\ 0, \text{ if } (i,j) = (1,1) \end{cases}, t_{ij} = \begin{cases} m_{ij}, \text{ if } (i,j) \neq (n,n) \\ 0, \text{ if } (i,j) = (n,n) \end{cases}.$$

Lemma 2.3. Let $M = (m_{ij})$ be a real matrix of order $n \geq 3$ and $m_{11}m_{nn} \neq 0$. Keeping the notations above, then

$$\det(M)\det(R) = \det(S)\det(T) - m_{11}m_{nn}\det(M_n^1)\det(M_1^n). \tag{17}$$

Proof. Set

$$F = \begin{pmatrix} 1 & \alpha_n & 0 \\ -\alpha_n^T & R & -\beta_n^T \\ 0 & \beta_n & 1 \end{pmatrix},$$

which is a matrix of order $n+2$, where $\alpha_n = (c, 0, \ldots, 0), \beta_n = (0, 0, \ldots, 0, d)$ are two vector with n entries, and $c^2 = m_{11}, d^2 = m_{nn}$.

By the Dodgson's determinant-evaluation rule,

$$\det(F)\det(F_{1(n+2)}^{1(n+2)}) = \det(F_1^1)\det(F_{n+2}^{n+2}) - \det(F_1^{n+2})\det(F_{n+2}^1). \quad (18)$$

It is not difficult to prove the followings:

$$\det(F) = \det(R + \alpha_n^T\alpha_n + \beta_n^T\beta_n) = \det(M), \quad (19)$$

$$\det(F_{1(n+2)}^{1(n+2)}) = \det(R), \quad (20)$$

$$\det(F_1^1) = \det(R + \beta_n^T\beta_n) = \det(S), \quad (21)$$

$$\det(F_{n+2}^{n+2}) = \det(R + \alpha_n^T\alpha_n) = \det(T), \quad (22)$$

$$\det(F_1^{n+2}) = -cd\det(R_1^n) = -cd\det(M_1^n), \quad (23)$$

$$\det(F_{n+2}^1) = -cd\det(R_n^1) = -cd\det(M_n^1). \quad (24)$$

Hence Eq. (17) is immediate from Eqs. (18)-(24) and the lemma thus holds. ■

Now, we can give the proofs of the main results.

Proof of Theorem 1.1. Note that (V_1, V_2) is the bipartition of G. If $|V_1| \neq |V_2|$, then $\det(A(G)) = 0$. It is not difficult to see that $C(G) = C(G - f - g) = C(G - f) = C(G - g) = C(G - u - x) = C(G - w - v) = 0$. Hence it suffices to consider the case of $|V_1| = |V_2| =: n$. Set $V_1 = \{v_1^{(1)}, v_2^{(1)}, \ldots, v_n^{(1)}\}, V_2 = \{v_1^{(2)}, v_2^{(2)}, \ldots, v_n^{(2)}\}$. Let $B = (b_{ij})$ be the bipartite adjacency matrix of G, where

$$b_{ij} = \begin{cases} 1 & \text{if } v_i^{(1)} v_j^{(2)} \text{ is an edge of } G, \\ 0 & \text{otherwise.} \end{cases}$$

Then

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

is the adjacency matrix of G. So, by Eq. (1),

$$(-1)^n C(G)^2 = \det(A(G)) = (-1)^n \det(B)^2, \tag{25}$$

which implies that

$$C(G) = \pm \det(B). \tag{26}$$

We can set $v_1^{(1)} = u, v_n^{(1)} = w, v_1^{(2)} = v, v_n^{(2)} = x$. Then $b_{11} = b_{nn} = 1$. Define three matrices $R = (r_{ij}), S = (s_{ij})$ and $T = (t_{ij})$ of order n from B such that

$$r_{ij} = \begin{cases} b_{ij}, \text{ if } (i,j) \neq (1,1), (n,n) \\ 0, \text{ if } (i,j) = (1,1), (n,n) \end{cases},$$

$$s_{ij} = \begin{cases} b_{ij}, \text{ if } (i,j) \neq (1,1) \\ 0, \text{ if } (i,j) = (1,1) \end{cases}, t_{ij} = \begin{cases} b_{ij}, \text{ if } (i,j) \neq (n,n) \\ 0, \text{ if } (i,j) = (n,n) \end{cases}.$$

By Lemma 2.3,

$$\det(B)\det(R) = \det(S)\det(T) - \det(B_n^1)\det(B_1^n). \tag{27}$$

It is not difficult to see that R, S, T, B_n^1 and B_1^n are the bipartite adjacency matrices of $G - f - g, G - f$, $G - g, G - v_1^{(2)} - v_n^{(1)}$ (i.e., $G - w - v$) and $G - v_1^{(1)} - v_n^{(2)}$ (i.e., $G - u - x$), respectively. Similarly,

$$C(G - f - g) = \pm \det(R), C(G - f) = \pm \det(S), \tag{28}$$

$$C(G - g) = \pm \det(T), C(G - w - v) = \pm \det(B_n^1), \tag{29}$$

$$C(G - u - x) = \pm \det(B_1^n). \tag{30}$$

By Eqs. (26)-(30), the theorem thus holds. ■

Proof of Theorem 1.2. Using a similar method to that in the proof of Theorem 1.1, we can give the proof of the theorem. Hence we omit the proof of Theorem 1.2. ■

3 Discussion

For the number of perfect matchings of a graph G, it satisfies a recurrence Eq. (4). Motivated by this result, Gutman obtained some similar formulas—the Gutman's forumae Eqs. (5)-(7), for the algebraic structure count of bipartite graphs. Based on the Dodgson's determinant-evaluation rule, the current author in this paper obtained a variant, i.e., three equations above Theorem 1.1, of the Gutman's formulas in [19], which is called the formulas for the vertex graphical condensation. In this paper, by using new two variants of the Dodgson's determinant-evaluation rule (i.e., Lemmas 2.2 and 2.3), we obtain two new variants of the Gutman's formulas, which are called the formulas for the edge graphical condensation and vertex-edge graphical condensation, i.e., Theorems 1.1 and 1.2.

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