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A Recurrence on the Algebraic Structure Count of Bipartite Graphs

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Abstract

Suppose that G is a connected bipartite graph with bipartition (U, V) and $f(G)$ be the algebraic structure count of G. Gutman [Note on algebraic structure count, *Z. Naturforsch.* **39a** (1984) 794–796.] proved that, if uv is an edge of G, then there exists an $\epsilon \in \{1, -1\}$ such that

$$f(G) = |f(G - uv) + \epsilon f(G - u - v)|. \qquad (i)$$

Ye [Further variants of Gutman's formulas, *MATCH Commun. Math. Comput. Chem.* **90** (2023) 235–245.] obtained a variant of the Gutman's formula above and proved that if $|U| = |V| = n$, then there exists a $\beta = (\nu_1, \nu_2, \ldots, \nu_m)$ satisfying $\nu_1, \nu_2, \ldots, \nu_m \in \{1, -1\}$ such that

$$(m - n)f(G) = \left| \sum_{i=1}^{m} \nu_i f(G - e_i) \right|, \qquad (ii)$$

where the sum ranges over all edges $e_1, e_2, \ldots, e_m$ of G.

Both formulae (i) and (ii) are linear recurrences. But it is difficult to determine $\epsilon = 1$ or -1 in (i) and $\nu_i = 1$ or -1 in (ii). In this paper, we obtain a quadratic recurrence of the algebraic structure count of G as follows.

$$(|E(G)| - 2n)f^2(G) = \sum_{uv \in E(G)} [f^2(G - uv) - f^2(G - u - v)], \quad (iii)$$

where the sum ranges over all edges of G. Meanwhile, we obtain a quadratic recurrence of the number of perfect matchings of G which is similar to formula (iii).

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1 Introduction

Suppose that G is a connected bipartite graph with bipartition (U, V) satisfying $|U| = |V| = n$ and $E(G)$ is the edge set of G. Let $U = \{u_1, u_2, \ldots, u_n\}$, $V = \{v_1, v_2, \ldots, v_n\}$. Define the biadjacency matrix $B_G = (b_{ij})_{n\times n}$ as

$$b_{ij} = \begin{cases} 1, & \text{if } u_i v_j \text{ is an edge of } G; \\ 0, & \text{otherwise.} \end{cases}$$

Hence the adjacency matrix of G can be expressed by

$$A_G = \begin{pmatrix} 0 & B_G \\ B_G^T & 0 \end{pmatrix}.$$

Obviously,

$$\det(A_G) = (-1)^n \det{}^2(B_G). \tag{1}$$

Wilcox, a theoretical organic chemist, defined the algebraic structure count of $G = (U, V)$ in [11,12], denoted by $f(G)$, as the difference between the number of so-called "even" and "odd" perfect matchings of G, which is equivalent to the absolute value of the determinant $\det(B_G)$. That is,

$$f(G) = |\det(B_G)|. \tag{2}$$

By Eq. (1),

$$\det(A_G) = (-1)^n f^2(G). \tag{3}$$

The algebraic structure count $f(G)$ has a closed relation with the thermodynamic stability of the corresponding molecular graphs and has important applications in theoretical organic chemistry [5,8,9,13,14]. On the further research on $f(G)$, see references [1–4, 6, 10, 15–17].

Let uv be an edge of G. Gutman [6] proved that one of the following relations holds.

$$f(G) = f(G - uv) + f(G - u - v), \tag{4}$$

$$f(G) = f(G - uv) - f(G - u - v), \tag{5}$$

$$f(G) = f(G - u - v) - f(G - uv). \tag{6}$$

Gutman's formulas above show that there exists an $\epsilon \in \{1, -1\}$ such that

$$f(G) = |f(G - uv) + \epsilon f(G - u - v)|. \tag{7}$$

Motivated by Eqs. (4)-(7), Ye [17] obtained a variant of Gutman's formulas and prove that there exist $\nu_i \in \{1, -1\}$ for $1 \leq i \leq m$ such that

$$(m - n)f(G) = \left| \sum_{i=1}^{m} \nu_i f(G - e_i) \right|, \tag{8}$$

where the sum ranges over all edges $e_1, e_2, \ldots, e_m$ of G.

Both formulas (7) and (8) are linear recurences. But as the authors in [6, 17] pointed out, it is very difficult to determine $\epsilon = 1$ or -1 in (7) and $\nu_i = 1$ or -1 in (8). In this paper, we obtain a quadratic recurrence on $f(G)$ and $\{f(G - uv), f(G - u - v) | uv \in E(G)\}$ as follows.

Theorem 1. *Let G be a connected bipartite graph with bipartition (U, V) satisfying $|U| = |V| = n$ and edge set $E(G)$. Then*

$$(|E(G)| - 2n)f^2(G) = \sum_{uv \in E(G)} [f^2(G - uv) - f^2(G - u - v)], \tag{9}$$

where the sum ranges over all edges of G.

On the other hand, Gutman and Hosoya [7] proved that the number of perfect matchings of G, denoted by $p(G)$, satisfies that

$$(|E(G)| - n)p(G) = \sum_{e \in E(G)} p(G - e). \tag{10}$$

Similarly, we can obtain the following result on $p(G)$.

Theorem 2. *Let G be a connected bipartite graph with bipartition (U, V) satisfying $|U| = |V| = n$ and edge set $E(G)$. Then*

$$(|E(G)| - 2n)p^2(G) = \sum_{uv \in E(G)} [p^2(G - uv) - p^2(G - u - v)], \qquad (11)$$

where the sum ranges over all edges of G.

We will give the proofs of Theorems 1 and 2 in the next section.

2 Proofs of main results

In order to prove Theorems 1 and 2, we first introduce some notations in linear algebra.

Let $M = (m_{ij})_{n\times n}$ be a matrix of order n. For any integers $1 \leq i_1 < i_2 < \ldots < i_k \leq n$ and $1 \leq j_1 < j_2 < \ldots < j_k \leq n$, let $M^{i_1,i_2,\ldots,i_k}_{j_1,j_2,\ldots,j_k}$ be the matrix obtained from M by deleting rows labelling $i_1, i_2, \ldots, i_k$ and columns labelling $j_1, j_2, \ldots, j_k$ of M.

Let $X = (x_{st})_{n\times n}$ be a symmetric matrix of order n over the complex field. Then $x_{st} = x_{ts}$ for any $1 \leq s, t \leq n$. For any $1 \leq i, j \leq n$, define a symmetric matrix $X_{[ij]} = (x^{ij}_{st})_{n\times n}$, where

$$x^{ij}_{st} = \begin{cases} x_{st}, & \text{if } (s,t) \neq (i,j) \text{ and } (s,t) \neq (j,i); \\ 0, & \text{otherwise.} \end{cases}$$

That is, $X_{[ij]} = X_{[ji]}$ is the symmetric matrix obtained from X by replacing the (i, j)-entry x_{ij} and the (j, i)-entry x_{ji} with 0. Obviously, if $x_{ij} = 0$, then $X = X_{[ij]} = X_{[ji]}$.

Now we can prove the following results which will play an important role in the proof of main results in this paper.

Lemma 1. *Let $X = (x_{st})_{n\times n}$ be a symmetric matrix of order n over the complex field and let $X_{[ij]}$ be defined as above. Then the determinant* $\det(X)$ *of X satisfies:*

$$(|I_i| - 2)\det(X) = \sum_{j \in I_i} \left[\det(X_{[ij]}) + x^2_{ij} \det(X^{i,j}_{i,j})\right], \qquad (12)$$

where $I_i = \{k | x_{ik} \neq 0,\ 1 \leq k \leq n\}$.

Proof. Note that, for any $1 \leq i \neq j \leq n$,

$$\begin{aligned}
&\det(X_{[ij]}) \\
&= \det(X) - (-1)^{i+j} x_{ij} \det(X_j^i) - (-1)^{i+j} x_{ji} \det(X_i^j) - x_{ij}^2 \det(X_{i,j}^{i,j}).
\end{aligned} \tag{13}$$

We have

$$\begin{aligned}
&\sum_{j=1}^{n} \det(X_{[ij]}) \\
=&\sum_{j=1}^{n} \det(X) - \sum_{j=1}^{n} (-1)^{i+j} x_{ij} \det(X_j^i) - \sum_{j=1}^{n} (-1)^{i+j} x_{ji} \det(X_i^j) \\
&- \sum_{j=1}^{n} x_{ij}^2 \det(X_{i,j}^{i,j}) \\
=&n \det(X) - 2\det(X) - \sum_{j=1}^{n} x_{ij}^2 \det(X_{i,j}^{i,j}) \\
=&(n-2)\det(X) - \sum_{j=1}^{n} x_{ij}^2 \det(X_{i,j}^{i,j}).
\end{aligned} \tag{14}$$

By Eq. (14),

$$\sum_{j \in I_i} \det(X_{[ij]}) + (n - |I_i|) \det(X) = (n-2)\det(X) - \sum_{j \in I_i} x_{ij}^2 \det(X_{i,j}^{i,j}). \tag{15}$$

Then

$$(|I_i| - 2) \det(X) = \sum_{j \in I_i} \left[\det(X_{[ij]}) + x_{ij}^2 \det(X_{i,j}^{i,j}) \right]. \tag{16}$$

The lemma thus follows. ■

Note that the permanent of a matrix $X = (x_{ij})_{n \times n}$ is defined as

$$\mathrm{per}(X) = \sum_{\alpha \in S_n} x_{1\alpha(1)} x_{2\alpha(2)} \dots x_{n\alpha(n)},$$

where α ranges over the set of the symmetric group of order n. Then we have a similar result to Lemma 1 as follows.

Lemma 2. *Let $X = (x_{st})_{n\times n}$ be a symmetric matrix of order n over the complex field and let $X_{[ij]}$ be defined as above. Then the permanent* $\mathrm{per}(X)$ *of X satisfies:*

$$(|I_i| - 2)\mathrm{per}(X) = \sum_{j\in I_i} \left[\mathrm{per}(X_{[ij]}) - x_{ij}^2 \mathrm{per}(X_{i,j}^{i,j})\right], \tag{17}$$

where $I_i = \{k | x_{ik} \neq 0,\ 1 \leq k \leq n\}$.

Proof. Note that, for any $i, j \in \{1, 2, \ldots, n\}$ and $i \neq j$,

$$\mathrm{per}(X_{[ij]}) = \mathrm{per}(X) - x_{ij}\mathrm{per}(X_j^i) - x_{ji}\mathrm{per}(X_i^j) + x_{ij}^2\mathrm{per}(X_{i,j}^{i,j}). \tag{18}$$

Similarly to the proof of Lemma 1, we obtain

$$\sum_{j=1}^{n} \mathrm{per}(X_{[ij]}) = (n-2)\mathrm{per}(X) + \sum_{j=1}^{n} x_{ij}^2 \mathrm{per}(X_{i,j}^{i,j}). \tag{19}$$

Then we have

$$\sum_{j\in I_i} \mathrm{per}(X_{[ij]}) + (n - |I_i|)\mathrm{per}(X) = (n-2)\mathrm{per}(X) + \sum_{j\in I_i} x_{ij}^2 \mathrm{per}(X_{i,j}^{i,j}). \tag{20}$$

Hence

$$(|I_i| - 2)\mathrm{per}(X) = \sum_{j\in I_i} \left[\mathrm{per}(X_{[ij]}) - x_{ij}^2 \mathrm{per}(X_{i,j}^{i,j})\right]. \tag{21}$$

The lemma thus follows. ■

Let G be a connected bipartite graph with bipartition (U, V) satisfying $|U| = |V| = n$, where $V(G)$ and $E(G)$ are the vertex set and edge set of G, respectively. Then the adjacency matrix A_G of G is a $2n \times 2n$ matrix.

Lemma 3. *Let G be a connected bipartite graph with bipartition (U, V) satisfying $|U| = |V| = n$. Then the algebraic structure count $f(G)$ of G satisfies:*

$$(d_G(u) - 2)f^2(G) = \sum_{v\in N_G(u)} \left[f^2(G - uv) - f^2(G - u - v)\right], \tag{22}$$

where $N_G(u)$ is the set of neighbours of the vertex u in G and $d_G(u) = |N_G(u)|$ is the degree of u.

Proof. For any vertex $u \in V(G)$, by Lemma 1,

$$(d_G(u) - 2)\det(A_G) = \sum_{v \in N_G(u)} \left[\det(A_{G-uv}) + \det(A_{G-u-v})\right]. \tag{23}$$

For any edge $uv \in E(G)$, by Eq. (3), we obtain

$$f^2(G) = (-1)^n \det(A_G), \tag{24}$$
$$f^2(G - uv) = (-1)^n \det(A_{G-uv}), \tag{25}$$
$$f^2(G - u - v) = (-1)^{n-1} \det(A_{G-u-v}). \tag{26}$$

Hence

$$(d_G(u) - 2)f^2(G) = \sum_{v \in N_G(u)} \left[f^2(G - uv) - f^2(G - u - v)\right], \tag{27}$$

the lemma holds. ■

Similarly, we can obtain the following result on $p(G)$.

Lemma 4. *Let G be a connected bipartite graph with bipartition (U, V) satisfying $|U| = |V| = n$. Then the number $p(G)$ of perfect matchings of G satisfies:*

$$(d_G(u) - 2)p^2(G) = \sum_{v \in N_G(u)} \left[p^2(G - uv) - p^2(G - u - v)\right], \tag{28}$$

where $N_G(u)$ is the set of neighbours of the vertex u in G and $d_G(u) = |N_G(u)|$ is the degree of u.

Proof. For any vertex $u \in V(G)$, by Lemma 2,

$$(d_G(u) - 2)\mathrm{per}(A_G) = \sum_{v \in N_G(u)} \left[\mathrm{per}(A_{G-uv}) - \mathrm{per}(A_{G-u-v})\right]. \tag{29}$$

For any edge $uv \in E(G)$, it is no difficult to show that

$$p^2(G) = \mathrm{per}(A_G), \tag{30}$$

$$p^2(G-uv) = \mathrm{per}(A_{G-uv}), \tag{31}$$

$$p^2(G-u-v) = \mathrm{per}(A_{G-u-v}). \tag{32}$$

Hence

$$(d_G(u)-2)p^2(G) = \sum_{v\in N_G(u)} \left[p^2(G-uv) - p^2(G-u-v)\right], \tag{33}$$

the lemma holds. ■

Proof of Theorem 1. By Lemma 3, we have

$$\sum_{u\in V(G)} (d_G(u)-2)f^2(G) = \sum_{u\in V(G)} \sum_{v\in N_G(u)} \left[f^2(G-uv) - f^2(G-u-v)\right]. \tag{34}$$

Note that $\sum_{u\in V(G)} d_G(u) = 2|E(G)|$. Then

$$(2|E(G)| - 4n)f^2(G) = 2\sum_{uv\in E(G)} \left[f^2(G-uv) - f^2(G-u-v)\right], \tag{35}$$

i.e.,

$$(|E(G)| - 2n)f^2(G) = \sum_{uv\in E(G)} \left[f^2(G-uv) - f^2(G-u-v)\right]. \tag{36}$$

Hence we have finished the proof of Theorem 1.

Proof of Theorem 2. By Lemma 4, we have

$$\sum_{u\in V(G)} (d_G(u)-2)p^2(G) = \sum_{u\in V(G)} \sum_{v\in N_G(u)} \left[p^2(G-uv) - p^2(G-u-v)\right]. \tag{37}$$

Similarly to the proof of Theorem 1, we obtain

$$(|E(G)| - 2n)p^2(G) = \sum_{uv\in E(G)} \left[p^2(G-uv) - p^2(G-u-v)\right]. \tag{38}$$

Hence Theorem 2 holds.

3 Discussions

In this paper, we obtain two identities Eqs. (12) and (17), one is related to the determinants, and the other is related to the permanents. Using these two identities, we obtain two quadratic recurrences of the algebraic structure count and the number of perfect matchings of G, respectively.

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