Invariant factors of graphs associated with hyperplane arrangements

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Abstract

A matrix called Varchenko matrix associated with a hyperplane arrangement was defined by Varchenko in 1991. Matrices that we shall call q-matrices are induced from Varchenko matrices. Many researchers are interested in the invariant factors of these q-matrices. In this paper, we associate this problem with a graph theoretic model. We will discuss some general properties and give some methods for finding the invariant factors of q-matrices of certain types of graphs. The proofs are elementary. The invariant factors of complete graphs, complete bipartite graphs, even cycles, some hexagonal systems, and some polygonal trees are found.

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1. Introduction and background

Let \( \mathcal{H} = \{H_1, \ldots, H_t\} \) be an arrangement (or a configuration) of hyperplanes in \( \mathbb{R}^n \). Let \( r(\mathcal{H}) = \{R_1, \ldots, R_m\} \) be the sets of regions in the complement of the union of elements in \( \mathcal{H} \). For any regions \( R_i, R_j \in r(\mathcal{H}) \), let \( s(R_i, R_j) \) be the set of hyperplanes in \( \mathcal{H} \) which separate \( R_i \) from \( R_j \). Varchenko in [17] defined a matrix \( B = B(\mathcal{H}) \), with rows and columns indexed by the regions in \( r(\mathcal{H}) \) and \( (B)_{i,j} = \prod_{H \in s(R_i, R_j)} a_H \), where \( a_H \) is an indeterminate called the weight assigned to the hyperplane \( H \). \( B \) is called Varchenko matrix of the arrangement \( \mathcal{H} \).

Varchenko matrix first appeared in the work of Schechtman and Varchenko [7]. That paper was initially a chapter of [18]. The nullspaces of the Varchenko matrices for some values of the indeterminates \( a_H \)’s are of particular interest [17]. When we let \( a_H = q \) for all \( H \in \mathcal{H} \), then the Varchenko matrix becomes a matrix over \( \mathbb{Q}[q] \) (sometimes we consider this matrix over the field \( \mathbb{C}(q) \)), which is an Euclidean domain. Let us call this matrix a q-matrix. We can define the Smith normal form of the q-matrix [16]. Entries appearing in the diagonal of a Smith normal form of a matrix are called invariant factors. Applications of invariant factors of a q-matrix can be found in [3].

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Smith normal form was discovered by H.J.S. Smith.

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We are going to associate the \( q \)-matrices of hyperplane arrangements with a graph theoretic model. All graphs under consideration are finite, connected and simple. Any undefined graph theoretic and algebraic terminologies and notations used in this paper may be found in any textbook, for example [1,5].

Let \( \mathbf{S} \) be an arrangement of hyperplanes in \( \mathbb{R}^n \), \( r(\mathbf{S}) \) be defined above and \( B \) be the Varchenko matrix of \( \mathbf{S} \). If we set \( a_H = q \) for all \( H \in \mathbf{S} \), then \( B \) becomes a matrix, say \( Q \), whose entries are in \( \mathbb{Q}[q] \) (in fact in \( \mathbb{Z}[q] \)). For any \( R_i, R_j \in r(\mathbf{S}) \), the \((i, j)\)-entry (or the \((R_i, R_j)\)-entry) of \( Q \) is given by \( Q_{i,j} = q^{n(R_i, R_j)} \), where \( n(R_i, R_j) \) is the number of hyperplanes in \( \mathbf{S} \) which separate \( R_i \) from \( R_j \). We define a graph \( G(\mathbf{S}) \) whose vertex set is \( r(\mathbf{S}) \). Two vertices (regions) are adjacent if their closures have an \((n - 1)\)-dimensional common boundary. \( G(\mathbf{S}) \) is called the graph of \( \mathbf{S} \). It is easy to see that \( G(\mathbf{S}) \) contains no odd cycles, i.e., \( G(\mathbf{S}) \) is a connected bipartite graph. Moreover, \( G(\mathbf{S}) \) contains a cycle unless all the hyperplanes are parallel. For any \( R_i, R_j \in r(\mathbf{S}) = V(G(\mathbf{S})) \), let \( x_i \in R_i \) and \( y_j \in R_j \). Any connected curve joining \( x \) and \( y \) must pass through all the hyperplanes in \( \mathbf{S} \) which separate \( R_i \) and \( R_j \) at least once and there is a connected curve joining \( x \) and \( y \) passing through those hyperplanes exactly once. Thus \( n(R_i, R_j) \) is the distance between \( R_i \) and \( R_j \) in \( G(\mathbf{S}) \).

Let \( D_G = (d_{i,j}) \) (or simply \( D \)) be the distance matrix of a graph \( G \) under an ordering of vertices. Let \( Q_G(q) = \left( q^{d_{i,j}} \right) \) (or simply \( Q(q) \), \( Q_G \) or \( Q \); sometimes denoted as \( q^D \)), where \( q \) is an indeterminate. \( Q_G(q) \) is called the \( q \)-matrix of \( G \) (it is unique up to isomorphism). If \( G \) is a graph of an arrangement of hyperplanes \( \mathbf{S} \), then \( Q_G(q) \) is the \( q \)-matrix of the Varchenko matrix of \( \mathbf{S} \). We call it the \( q \)-matrix of \( \mathbf{S} \).

In this paper, we shall determine the invariant factors of \( q \)-matrices of some graphs, which in particular give the determinants of those \( q \)-matrices. This is important for applications to quantum groups and Knizhnik–Zamolodchikov equations [2,3,7,17,18]. The invariant factors of complete graphs, complete bipartite graphs, even cycles, hexagonal graphs and polygonal trees are described in Sections 3, 5 and 6. Some relationships between \( q \)-matrix of a graph and its subgraphs are established in Section 4. All the proofs are elementary.

### 2. Examples and invariant factor of a graph

In this section, we shall give some examples of hyperplane arrangements and their associated graphs and \( q \)-matrices. Some basic properties of \( q \)-matrices of graphs are given.

**Example 2.1.** Let \( \mathbf{S} = \{H_1, H_2, H_3\} \) be an arrangement of hyperplanes in \( \mathbb{R}^2 \) and \( r(\mathbf{S}) = \{R_1, R_2, \ldots, R_7\} \) described in Fig. 1 (a). This example is selected from Example 1.1 of [3]. The graph \( G = G(\mathbf{S}) \) is described in Fig. 1 (b) and \( Q_G \) is given by

\[
Q_G = \begin{pmatrix}
1 & q & q^2 & q^3 & q^2 & q & q \\
q & 1 & q & q^2 & q^3 & q^2 & q \\
q^2 & q & 1 & q & q^2 & q & q \\
q^3 & q^2 & q & 1 & q & q^2 & q \\
q^2 & q^3 & q^2 & q & 1 & q & q \\
q & q^2 & q^3 & q^2 & q & 1 & q \\
q^2 & q & q^2 & q & q^2 & q & 1
\end{pmatrix}.
\]

**Example 2.2.** For \( 1 \leq i \leq n \), let \( O_i = \{(x_1, \ldots, x_n) \in \mathbb{R}^n \mid x_i = 0\} \). Let \( \mathcal{S}_n = \{O_1, \ldots, O_n\} \) (see [2,3]). Then \( r(\mathcal{S}_n) \) has \( 2^n \) regions and can be indexed by vectors \( \alpha = (a_1, \ldots, a_n) \), where \( a_i \) is either 1 or \(-1\). \( \alpha \) corresponds to the region \( R_2 \) which contains all points \( (x_1, \ldots, x_n) \) where \( x_i < 0 \) if and only if \( a_i = -1 \). Then the graph of \( \mathcal{S}_n \) is isomorphic to the \( n \)-cube.

**Example 2.3.** For \( 1 \leq i < j \leq n \), let \( H_{i,j} = H_{j,i} = \{(x_1, \ldots, x_n) \in \mathbb{R}^n \mid x_i = x_j\} \). Let \( \mathcal{M}_n = \{H_{i,j} \mid 1 \leq i < j \leq n\} \) (see [2,3]). It is called the *braid arrangement*. Then \( r(\mathcal{M}_n) \) has \( n! \) regions and can be indexed by permutations \( \sigma \in S_n \). \( \sigma \) corresponds to the region \( R_0 = \{(x_1, \ldots, x_n) \mid x_{\sigma(1)} < x_{\sigma(2)} < \cdots < x_{\sigma(n)}\} \). Then the graph of \( \mathcal{M}_n \) is isomorphic to the Cayley graph \( I(S_n, T) \), where \( T \) is the generating set which is the set of all transpositions.

Let \( Q_G(q) = Q \) be a \( q \)-matrix of a connected graph \( G \) of order \( n \). Then \( Q \) is an \( n \times n \) (symmetric) matrix over \( \mathbb{Q}[q] \). There exist two invertible matrices \( U \) and \( V \) over \( \mathbb{Q}[q] \) such that \( UQV = diag(s_1(q), s_2(q), \ldots, s_n(q)) = S(q) \) and \( s_j(q) |_{s_{j+1}(q)} \), \( 1 \leq i \leq n - 1 \), where \( s_j(q) \in \mathbb{Q}[q] \). Since \( Q(z) \) is not a zero matrix for any \( z \in \mathbb{C} \), rank \( Q(z) \geq 1 \). Hence \( s_j(q) \in \mathbb{Q} \) (it can be assumed to be 1). \( S(q) \) is called the Smith normal form of \( Q \) and the polynomials \( s_j(q) \) are called the invariant factors of \( Q \) (see [4, p. 79–84, 5, p. 175–179, 6, p. 63]). \( S(q) \) and \( s_j(q) \) are also called the Smith normal form and the invariant factors of \( G \), respectively. We shall denote the *multiset* of all the invariant factors of \( G \) by \( \text{Inv}(G) \). From now on, all sets are considered as multisets and all the set operations are considered as multiset operations.
Let $G$ be any graph. Then

$$\text{Inv}(G) = \{1, (1 - q^2), (1 - q^2)^2, (1 - q^2)^3, (1 - q^2)^4, (1 - q^2)^5\}.$$ 

**Theorem 2.1.** Let $G$ be any graph. Then $1 - q$ is a divisor of each invariant factor of $G$ except the first one.

**Proof.** It follows from rank $Q_G(1) = 1$. □

**Theorem 2.2.** Let $G$ be a bipartite graph. If $f(q)$ is an irreducible divisor of an invariant factor of $G$ with multiplicity $\alpha$, then $f(-q)$ is an irreducible divisor of the same invariant factor with the same multiplicity $\alpha$.

**Proof.** Let $(X, Y)$ be the bipartition of $G$. Let $D = \begin{pmatrix} A_1 & B \\ B^T & A_2 \end{pmatrix}$, for some $A_1 \in M_m(Z)$, $A_2 \in M_n(Z)$ and $B \in M_{m,n}(Z)$. Since any entry of $A_1$ or $A_2$ is even and any entry of $B$ is odd, $Q(-q) = \begin{pmatrix} qA_1 & -(qB)^T \\ -(qB) & qA_2 \end{pmatrix}$. Let

$$P = \begin{pmatrix} I_m & O_{m,n} \\ O_{n,m} & -I_n \end{pmatrix},$$

where $I_t$ is the $t \times t$ identity matrix and $O_{m,n}$ is the $m \times n$ zero matrix. Then $PQ(q)P = Q(-q)$. Therefore $Q(q)$ and $Q(-q)$ have the same invariant factors. □

**Corollary 2.3.** Let $G$ be a bipartite graph. Every invariant factor of $G$ is of the form $f(q^2)$ for some $f(q) \in \mathbb{Q}[q]$. Hence $1 - q^2$ is a divisor of each invariant factor except the first one.

**Corollary 2.4.** Let $G$ be a bipartite graph. If $f(q)$ is an eigenvalue of $Q_G$ for some expression $f$ then so is $f(-q)$.

**Proof.** Since $P$, defined in the proof of Theorem 2.2, is symmetric and orthogonal, the corollary follows. □

For any graph $G$, there are some questions:

1. What is the determinant of $Q_G$?
2. What are the multiplicities of $1 - q$ and $1 + q$ in the invariant factors of $G$, respectively?
3. What is the spectrum of $Q_G$?
4. What is the Smith normal form of $G$?

There is a well-known method for computing the invariant factors of an $m \times n$ matrix over a principal ideal domain. This method can be found in many linear algebra or algebra textbooks, for example [5, p. 175–179]. Before we state that theorem, we have to introduce some notation and terminology. Let $A$ be an $m \times n$ matrix over a principal ideal domain, $r_1 < \cdots < r_t$, $c_1 < \cdots < c_t$, $t \leq \min(m, n)$. Let $A = \begin{pmatrix} r_1 & \cdots & r_t \\ c_1 & \cdots & c_t \end{pmatrix}$ denote the $t \times t$ submatrix obtained from $A$ by deleting all rows except rows $r_1, \ldots, r_t$ and deleting all columns except columns $c_1, \ldots, c_t$. If $(r_1, \ldots, r_t) = (c_1, \ldots, c_t)$ then we simply denote it by $A[r_1 \cdots r_t]$. The determinant of $A = \begin{pmatrix} r_1 & \cdots & r_t \\ c_1 & \cdots & c_t \end{pmatrix}$ is called a $t$-rowed minor of $A$. Two matrices $A$ and $B$ over a ring $R$ are called equivalent if there are two invertible matrices $U$ and $V$ over $R$ such that $B = UAV$. 

![Image](image.png)

Fig. 1. (a) A hyperplane arrangement. (b) The graph of the arrangement.
Theorem 2.5. Let $A$ be an $m \times n$ matrix over a principal ideal domain $\mathbb{D}$ and suppose that the rank of $A$ is $r$. Suppose $s_1, s_2, \ldots, s_r$ are the nonzero invariant factors of $A$. For each $i$, $1 \leq i \leq r$, let $A_i$ be the g.c.d. of all the $i$-rowed minors of $A$. Then any set of invariant factors of $A$ differ by unit multipliers from the elements $s_1 = A_1^{-1} s_2 = A_2 A_1^{-1} \ldots, s_r = A_r A_{r-1}^{-1}$.

Note that the invariant factors are invariant up to equivalence. Also the invariant factors do not change if we consider $A$ as a matrix over any principal ideal domain containing $\mathbb{D}$.

Let $A$ be an $n \times n$ matrix over a principal ideal domain. If $A$ is equivalent to a diagonal matrix $B$, then the multiset of entries in the diagonal of $B$ is called a pre-invariant factor set of $A$. If $A$ is a $q$-matrix of a graph $G$, then a pre-invariant factor set of $A$ is called a pre-invariant factor set of $G$. The elements of such set are called pre-invariant factors of $G$. Clearly this set is not unique.

Corollary 2.6. Let $A$ be an $m \times n$ matrix of rank $r$ over a principal ideal domain with nonzero invariant factors $s_1, s_2, \ldots, s_r$, where $s_i | s_{i+1}$, $1 \leq i \leq r - 1$. Suppose $\{f_1, \ldots, f_r, 0, 0, \ldots, 0\}$ is a pre-invariant factor set of $A$, where $f_i \neq 0$. Let $\phi$ be an irreducible factor of $f_1 f_2 \cdots f_r$. Denote the multiplicities of $\phi$ in the factors $f_j$’s by $0 \leq a_1 < a_2 < \cdots < a_r$. Then the multiplicity of $\phi$ in $s_j$ is $a_j$.

The sequence $a_1, a_2, \ldots, a_r$ is called the multiplicity sequence of $\phi$ with respect to $\{f_1, \ldots, f_r\}$. Because of Corollary 2.6, if the eigenvalues of $Q_A$ are polynomials of $q$ (over any extension field of $\mathbb{Q}$) then question 4 can be solved in principle.

3. Computational results of some bipartite graphs (I)

In this section, we give some examples to illustrate how to use Corollary 2.6 to find the invariant factors of some graphs.

3.1. Complete bipartite graphs

Let $J_{m,n}$ be the $m \times n$ matrix whose entries are $1$ and let $J_n = J_n,n$. The $q$-matrix of $K_{m,n}$ is

$$Q = \begin{pmatrix} q^2 J_m + (1 - q^2) I_m & q J_{m,n} \\ q J_{n,m} & q^2 J_n + (1 - q^2) I_n \end{pmatrix}.$$ 

After applying row operations $-q^2 r_1 + r_j$, $2 \leq j \leq m$; $-qr_1 + r_j$, $m + 1 \leq j \leq m + n$ and the same column operations, $Q$ becomes

$$Q_1 = \begin{pmatrix} 1 & O_{1,m-1} \\ O_{m-1,1} & (1 - q^2)(q^2 J_{m-1,n} + I_{m-1}) \end{pmatrix}.$$ 

For convenience, we omit to write the first row and first column of $Q_1$ and divide each of the remaining entries by $1 - q^2$. After applying row operations $-q r_{m+j} + r_i$, $1 \leq j \leq n$, $2 \leq i \leq m$ and the same column operations, the matrix becomes

$$Q_2 = \begin{pmatrix} (1 - n) q^2 J_{m-1,n} + I_{m-1} & O_{m-1,n} \\ O_{n,m-1} & I_n \end{pmatrix}.$$ 

We omit to write the last $n$ rows and columns of $Q_2$. Applying column operations $-c_3 + c_2$, $-c_4 + c_3$, $\ldots$, $-c_{m-1} + c_{m-2}$ and $r_3 + r_2$, $r_4 + r_3$, $\ldots$, $r_m + r_{m-1}$ in proper order, the matrix becomes

$$\begin{pmatrix} I_{m-2} \\ O_{1,m-2} \end{pmatrix} \begin{pmatrix} (1 - n) q^2 \\ 2(1 - n) q^2 \\ \vdots \\ (m - 2)(1 - n) q^2 \\ 1 + (m - 1)(1 - n) q^2 \end{pmatrix}.$$ 

After clearing the non-diagonal entries, the original matrix $Q$ becomes

$$\text{diag}[1, 1 - q^2, \ldots, 1 - q^2, (1 - q^2)(1 - (m - 1)(n - 1) q^2), 1 - q^2, \ldots, 1 - q^2].$$

Thus the invariant factors of $K_{m,n}$ are $1$, $1 - q^2$ [$(m + n - 2)$ times], $(1 - q^2)(1 - (m - 1)(n - 1) q^2)$. 

3.2. Composition of even cycles with null graphs

Let \(G\) and \(H\) be two graphs. The composition \(G \circ H\) of \(G\) with \(H\) is the graph with vertex set \(V(G) \times V(H)\) in which \((u_1, v_1)\) is adjacent to \((u_2, v_2)\) if and only if \(u_1u_2 \in E(G)\) or \(u_1 = u_2\) and \(v_1v_2 \in E(H)\).

Consider \(C_{2n} \circ N_n\), where \(C_{2n}\) is the cycle of order \(2n\) and \(N_n\) is the null graph of order \(n\). We write the vertex set of \(C_{2n} \circ N_n\) as \(\mathbb{Z}_n \times \mathbb{Z}_2\), where \(\mathbb{Z}_n = \{i, j\} | 0 \leq i, j \leq n - 1\) and \(\mathbb{Z}_2 = \{1, 2\}\). Let \(G\) be any field. Let \(\beta = (b_0, \ldots, b_{n-1}) \in \mathbb{F}^n\) and \(R(\beta)\) be the \(n \times n\) right cyclic (circulant) matrix whose first row is \(\beta\). It is known that (see [8]) the spectrum of \(R(\beta)\) is

\[
\{ n-1 \text{ times} \left\{ \sum_{j=0}^{n-1} b_j, \sum_{j=0}^{n-1} b_j \zeta^j, \sum_{j=0}^{n-1} b_j \zeta^{2j}, \ldots, \sum_{j=0}^{n-1} b_j \zeta^{(n-1)j} \right\} \},
\]

where \(\zeta\) is a primitive \(n\)th root of unity over \(\mathbb{F}\).

Now we come back to consider the graph \(G = C_{2n} \circ N_n\). If we arrange the vertices in lexicographic order (0 is the first), then the distance matrix of \(G\) is a right cyclic matrix of order \(2sn\) whose first row is

\[
\begin{align*}
\alpha &= (a_0, a_1, \ldots, a_{2sn-1}), \\
&= (0, 1, 2, \ldots, s, 3, 2, 1, \ldots, (2, 1, 2, 3, \ldots, s, 3, 2, 1)) \\
&\text{\(n-1\) times} \left\{ \sum_{j=0}^{2sn-1} a_j, \sum_{j=0}^{2sn-1} a_j \zeta^j, \sum_{j=0}^{2sn-1} a_j \zeta^{2j}, \ldots, \sum_{j=0}^{2sn-1} a_j \zeta^{(2sn-1)j} \right\} ,
\end{align*}
\]

where \(\zeta\) is a primitive \(2sn\)th root of unity over \(\mathbb{C}\). That is, if we let \(f_{s,n}(q, \lambda) = \sum_{j=0}^{2sn-1} a_j \lambda^j \in \mathbb{C}[q, \lambda]\), then the spectrum of \(Q_G\) is \(\{ f_{s,n}(q, \zeta^k) \} | 0 \leq k \leq 2sn - 1\). It is a pre-invariant factor set of \(G\).

First we assume \(s \geq 2\). For \(i \notin \{0, 2, s\}\), if \(a_k = i\) then \(k = sj + i\) for some \(0 \leq j \leq n\). If \(a_k = 2\) then \(k = sj + 2, 2s j - 2\) or \(2sj'\) for some \(0 \leq j' \leq n, 1 \leq j' \leq n - 1\). Thus when \(i \notin \{0, 2, s\}\) the coefficient of \(q^i\) of \(f_{s,n}(q, \zeta^k)\) is

\[
\sum_{j=0}^{n-1} \zeta^{2skj+ki} + \sum_{j=1}^{n-1} \zeta^{2skj-ki} = (\zeta^{ki} + \zeta^{-ki}) \sum_{j=0}^{n-1} \zeta^{2skj}
\]

The coefficient of \(q^s\) of \(f_{s,n}(q, \zeta^k)\) is

\[
\sum_{j=0}^{n-1} \zeta^{2skj+ks} = \zeta^{ks} \sum_{j=0}^{n-1} \zeta^{2skj}
\]
The coefficient of $q^2$ of $f_{s,n}(q, \zeta^k)$ is
\[
\sum_{j=0}^{n-1} \zeta^{2skj+2k} + \sum_{j=1}^{n} \zeta^{2skj-2k} + \sum_{j=1}^{n-1} \zeta^{2skj} = -1 + (\zeta^{2k} + \zeta^{-2k} + 1) \sum_{j=0}^{n-1} \zeta^{2skj}.
\]

It is known that
\[
\sum_{j=0}^{n-1} \zeta^{2skj} = \begin{cases} 
0 & \text{if } k \not\equiv 0 \pmod{n}, \\
1 & \text{if } k \equiv 0 \pmod{n}.
\end{cases}
\]

Therefore, for $k \not\equiv 0 \pmod{n}$, $f_{s,n}(q, \zeta^k) = 1 - q^2$; and for $0 \leq k \leq 2s - 1$,
\[
f_{s,n}(q, \zeta^{nk}) = 1 + (n-1)q^2 + (-1)^k nq^x + \sum_{i=1}^{s-1} (\zeta^{nki} + \zeta^{-nki})q^i = 1 - 2n + (n-1)q^2 + (-1)^k nq^x + n[1 - (-1)^k q^x] \left[ \frac{1}{1 - \zeta^{nk}q} + \frac{1}{1 - \zeta^{-nk}q} \right].
\]

(3.2)

In particular,
\[
f_{s,n}(q, 1) = 1 + (n-1)q^2 + 2n \sum_{i=1}^{s-1} q^i + nq^x = (1 + q) \left[ 1 + (n-1)q + n \sum_{i=1}^{s-1} q^i \right]
\]

and $f_{s,n}(1, 1) \neq 0$. Clearly, $f_{s,n}(q, \zeta^k) = f_{s,n}(q, \zeta^{2sn-k})$, i.e., $f_{s,n}(q, \zeta^k) \in \mathbb{R}[q]$.

If $s = 2$ then the coefficient of $q^2$ of $f_{2,n}(q, \zeta^k)$ is
\[
\sum_{j=1}^{2n-1} \zeta^{2skj} = -1 + \sum_{j=0}^{2n-1} \zeta^{2skj}.
\]

Thus $f_{2,n}(q, 1) = 1 + 2nq + (2n-1)q^2 = (1 + q)[1 + (2n-1)q]$; $f_{2,n}(q, \zeta^k) = 1 - q^2$ if $k \not\equiv 0 \pmod{n}$; and $f_{2,n}(q, \zeta^n) = 1 - q^2 = f_{2,n}(q, \zeta^{3n})$, $f_{2,n}(q, \zeta^{2n}) = 1 - 2nq + (2n-1)q^2 = (1 - q)[1 - (2n-1)q]$.

Example 3.1. Let $s = 4$ and $n = 2$, i.e., $G = C_4 \circ N_2$.

For brevity’s sake, we write $f$ for $f_{4,2}$.

\begin{align*}
 f(q, 1) &= 1 + 4q + 5q^2 + 4q^3 + 2q^4 = (1 + q)(1 + 3q + 2q^2 + 2q^3); \\
f(q, \zeta^k) &= 1 - q^2 \text{ if } k \text{ is odd, } 1 \leq k \leq 15; \\
f(q, \zeta^2) &= f(q, \zeta^{14}) = 1 + 2(\zeta^2 + \zeta^{-2})q + q^2 + 2(\zeta^6 + \zeta^{-6})q^3 - 2q^4 = (1 - q^2)(1 + \sqrt{2}q)^2; \\
f(q, \zeta^4) &= f(q, \zeta^{12}) = 1 - 3q^2 + 2q^4 = (1 - q^2)(1 - 2q^2); \\
f(q, \zeta^6) &= f(q, \zeta^{10}) = 1 + 2(\zeta^6 + \zeta^{-6})q + q^2 + 2(\zeta^2 + \zeta^{-2})q^3 - 2q^4 = (1 - q^2)(1 - \sqrt{2}q)^2; \\
f(q, \zeta^8) &= f(q, -1) = 1 - 4q + 5q^2 - 4q^3 + 2q^4 = (1 - q)(1 - 3q + 2q^2 - 2q^3).
\end{align*}

By applying Corollary 2.6,
\[
\text{Inv}(C_4 \circ N_2) = \{1, (1 - q^2), \ldots, (1 - q^2)^{11}\}, \quad (1 - q^2)(1 - 2q^2)^2, \quad (1 - 2q^2)(1 - 2q^2)^2, \quad (1 - 2q^2)(1 - 2q^2)^2(1 - 2q^2)^2(1 - 4q^2).
\]

We want to know whether $q = 1$ or $q = -1$ is a multiple root of $f_{s,n}(q, \zeta^k)$. Since $f_{s,n}(-q, \zeta^k) = f_{s,n}(q, \zeta^{n(k+s)})$ and $f_{s,n}(q, \zeta^k) = 1 - q^2$ if $k \not\equiv 0 \pmod{n}$, we only need to consider the multiplicity of $q = 1$ in $f_{s,n}(q, \zeta^{nk})$ when $1 \leq k \leq 2s - 1$ (1 is not a root of $f_{s,n}(q, 1)$).
For $1 \leq k \leq 2s - 1$, from (3.2) we have $f_{s,n}(1, \zeta^{nk}) = 0$ and
\[
 f'_{s,n}(1, \zeta^{nk}) = 2n - 2 + \frac{n[1 - (1)^k]}{\cos \frac{k\pi}{s} - 1} = \begin{cases} 
 2n - 2 + \frac{2n - 2}{\cos \frac{k\pi}{s} - 1} & \text{if } k \text{ is even,} \\
 2n - 2 + \frac{2n}{\cos \frac{k\pi}{s} - 1} & \text{if } k \text{ is odd,}
\end{cases}
\]
where $f'$ is the derivative of $f$ with respect to $q$. Thus we have the following lemma.

**Lemma 3.1.** For $1 \leq k \leq 2s - 1$, 1 is a double root of $f_{s,n}(q, \zeta^{nk})$ if and only if either $k$ is even and $n = 1$, or $k$ is odd and $\cos \frac{k\pi}{s} = \frac{1}{1-n}$.

**Proof.** From the previous paragraph we know that 1 is a multiple root of $f_{s,n}(q, \zeta^{nk})$ if and only if when $k$ is even and $n = 1$, or $k$ is odd and $\cos \frac{k\pi}{s} = \frac{1}{1-n}$.

\[
 f''(1, \zeta^{nk}) = 2(n - 1) + \frac{2n(1)(k+1) - n + (1)^k n}{\cos \frac{k\pi}{s} - 1} = \begin{cases} 
 2(n - 1) + \frac{2n(1 + \cos \frac{k\pi}{s})}{1-\cos \frac{k\pi}{s}} & \text{if } k \text{ is even,} \\
 2(n - 1) + \frac{2n-2n\cos \frac{k\pi}{s}}{1-\cos \frac{k\pi}{s}} & \text{if } k \text{ is odd,}
\end{cases}
\]

where $f''$ is the second derivative of $f$ with respect to $q$.

If $k$ is even, then clearly $f''(1, \zeta^{nk}) > 0$. If $k$ is odd, then 1 is a multiple root only if when $\cos \frac{k\pi}{s} = \frac{1}{1-n}$. In this case $f''(1, \zeta^{nk}) = 2(n - 1)(2 - s)$. If $f''(1, \zeta^{nk}) = 0$ then $s = 2$ and then $k = 1$. But this is not a case. □

**Corollary 3.2.** 1 is a double root of $f_{s,n}(q, -1)$ if and only if either $n = 1$ and $s$ is even, or $n = 2$ and $s$ is odd.

**Corollary 3.3.** For $0 \leq k \leq 2s - 1$ and $k \neq s$, $-1$ is a double root of $f_{s,n}(q, \zeta^{nk})$ if and only if either $k + s$ is even and $n = 1$, or $k + s$ is odd and $\cos \frac{k\pi}{s} = \frac{1}{n-1}$.

**Corollary 3.4.** $-1$ is a double root of $f_{s,n}(q, 1)$ if and only if either $n = 1$ and $s$ is even, or $n = 2$ and $s$ is odd.

By applying Corollary 2.6, when $n = 2$ and $s$ is even, the multiplicities of $1 - q^2$ in the invariant factors are $0, 1, \ldots, 1$; when $n = 2$ and $s$ is odd, the multiplicities of $1 - q^2$ are $0, 1, 1, 2$. For $n \geq 3$, if $\cos \frac{k\pi}{s}$ has a solution $k$ which is odd (in this case $2s - k$ is also a solution and that equation has at most 2 solutions) then the multiplicities of $1 - q^2$ in the invariant factors are $0, 1, \ldots, 1, 2, 2$, otherwise they are $0, 1, \ldots, 1$. In general, the invariant factors of $C_{2s} \circ N_q$ seem difficult to express when $n \geq 2$. For $n = 1$, they can be expressed. We will consider this case in the following subsection.

### 3.3. Even cycles

The invariant factors of even cycle $C_{2s}$ were computed in [2, Theorem 5.2]. In this subsection we shall use an elementary method to compute the invariant factors of $C_{2s}$. $C_{2s}$ is a special case of $C_{2s} \circ N_q$ when $n = 1$. We try to factorize the polynomials $f_{s,1}(q, \zeta^k)$. Note that $\deg(f_{s,1}) = s$. Suppose $\pm k + j \neq 0 \pmod{2s}$ and $k + j$ is even. For $0 \leq j \leq 2s - 1$,
\[
 f_{s,1}(\zeta^j, \zeta^k) = 2 + \sum_{i=0}^{s-1} \zeta^{(k+j)i} + \zeta^{(k-j)i} = \sum_{i=0}^{s-1} \zeta^{(k+j)i} + \sum_{i=0}^{s-1} \zeta^{(k-j)i}.
\]

Since $\sum_{i=0}^{s-1} \zeta^{(k+j)i} = \sum_{i=0}^{s-1} \zeta^{(k-j)i} = \sum_{i=0}^{s-1} \zeta^{(k+j)i} = \sum_{i=0}^{s-1} \zeta^{(k-j)i} = 0$. Similarly, $\sum_{i=0}^{s-1} \zeta^{(k-j)i} = 0$.

Thus $f_{s,1}(\zeta^j, \zeta^k) = 0$ when $\pm k + j \neq 0 \pmod{2s}$ and $k + j$ is even.

For a fixed $k$ there are $s - 2$ solutions for $j$. Let us consider the particular case that both $s$ and $k$ are even. There are $s - 2$ possibilities for $j$ (including $j = 0$ and $j = s$) such that $f_{s,1}(\zeta^j, \zeta^k) = 0$. In this case $q = 1$ and $q = -1$ are double roots of $f_{s,1}(q, \zeta^k)$. So we have found all roots of $f_{s,1}(q, \zeta^k)$. Similarly, we can find all roots of $f_{s,1}(q, \zeta^{-k})$ for the other cases. Combining the results above, we have the multiplicity sequences of irreducible factors of $f_{s,1}(q, \zeta^k)$'s with respect to the spectrum of $Q_{C_{2s}}$. 


as follows:

\[
\begin{array}{cc}
\text{times} & \text{times} \\
\text{s} & \text{s-1} \\
1-q & 0, 1, \ldots, 1, 2, \ldots, 2 .
\end{array}
\]

\[
\begin{array}{cc}
\text{j} & \text{f} \\
\neq 0 & \text{or } s, \quad \zeta^j = q : 0, \ldots, 0, 1, \ldots, 1 .
\end{array}
\]

The sequence of \(1+q\) is same as that of \(1-q\). Therefore we have the following result.

**Theorem 3.5.** The invariant factor set of \(C_{2s}\) is

\[
\begin{array}{cc}
\text{s times} & \text{s-2 times} \\
1, (1-q^2), \ldots, (1-q^2), & (1-q^2)(1-q^{2s}), \ldots, (1-q^2)(1-q^{2s}).
\end{array}
\]

Note that one can use the character theory of the cyclic group to establish Theorem 3.5.

4. Reductive methods

The natural question to ask is: can we find the invariant factors of a graph \(G\) if the invariant factors or pre-invariant factors of some subgraphs of \(G\) are known? In other word, can we reduce the problem of finding invariant factors of \(G\) to some of its subgraphs? Note that, suppose that \(H\) and \(K\) are subgraphs of \(G\). The definitions of the union \(H \cup K\) and the intersection \(H \cap K\) of \(H\) and \(K\) are referred to [1]. We have some results below.

**Theorem 4.1.** Let \(H\) and \(K\) be two subgraphs of \(G\) such that \(G = H \cup K\) and \(H \cap K \cong P_2\), the path of order 2. If \(H\) is bipartite, then Inv\((K)\) \(\cup\) Inv\((H)\) \(\setminus\) \{1, 1 \(- q\) \} is a pre-invariant factor set of \(G\).

**Proof.** Let \(uw\) be the common edge of \(H\) and \(K\). Let \(U = \{x \in V(H) \setminus \{u, w\} \mid d(x, u) < d(x, w)\}\) and \(W = \{y \in V(H) \setminus \{u, w\} \mid d(y, u) < d(y, w)\}\), where \(d(x, y)\) denotes the distance between vertices \(x\) and \(y\). Clearly \(U\) and \(W\) are disjoint. Since \(H\) is bipartite \(U \cup W = V(H) \setminus \{u, w\}\). Note that if \(d(z, u) < d(z, w)\) where \(z \in V(G)\) then \(d(z, u) + 1 = d(z, w)\). It is easy to see that for any \(z \in V(K)\) and \(x \in U, d(x, z) = d(x, u) + d(u, z)\). Similarly, for any \(z \in V(K)\) and \(y \in W, d(y, z) = d(y, w) + d(w, z)\).

Let \(U = \{x_1, \ldots, x_s\}\) and \(W = \{y_1, \ldots, y_r\}\) and \(V(K) = \{u, w, z_1, \ldots, z_r\}\). We arrange the vertices in the following order \(x_1, \ldots, x_s, y_1, \ldots, y_r, u, w, z_1, \ldots, z_r\). Let \(D\) be the distance matrix of \(G\) under this vertex ordering. Note that \(D_H = D[x_1 \cdots x_s \ y_1 \cdots y_r \ u \ w]\) and \(D_K = [u \ w \ z_1 \cdots z_r]\) are distance matrices of \(H\) and \(K\), respectively. Namely

\[
D = \begin{pmatrix}
D_1 & A_{11} & A_{12} & B_1 \\
A_{11}^T & A_{21} & A_{22} & C \\
A_{21}^T & A_{22} & D_2 \\
B_1^T & B_2^T & C^T & D_2
\end{pmatrix}
\]

where \(D_1 \in M_{s+r}(\bar{Z}), D_2 \in M_r(\bar{Z}), A_{11}, A_{12} \in M_{s,1} \bar{Z}, A_{21}, A_{22} \in M_{r,1}(\bar{Z}), B_1 \in M_{s,r}(\bar{Z}), B_2 \in M_{r,s}(\bar{Z})\) and \(C \in M_{s+r}(\bar{Z})\). Moreover, \(A_{11} = d(x_1, u), (A_{12})_j = d(x_j, u), (A_{21})_i = d(y_1, u), (A_{22})_j = d(y_j, u), (B_1)_i = d(x_1, u) + d(u, z_k),\)

\((B_2)_j = d(y_j, u) + d(w, z_k), C_{1k} = d(u, z_k)\) and \(C_{2k} = d(w, z_k)\). Then \(A_{11} + J_{s,1} = A_{12}\) and \(A_{22} + J_{r,1} = A_{21}\).

Let \(Q = q^D\).

**Step 1:** Do the row operations \(-q^{d(x_i, u)}r_u + r_{x_i}, 1 \leq i \leq s\) and \(-q^{d(y_j, w)}r_w + r_{y_j}, 1 \leq j \leq t\), on \(Q\); and then do the same column operations.

Then \(Q\) becomes

\[
Q_1 = \begin{pmatrix}
Q' & O_{s+t,2} & O_{s+t,r} \\
O_{2,s+t} & q & 1 \\
O_{r,s+t} & q^C & q^{D_2}
\end{pmatrix}.
\]

**Step 2:** Do \(-q^e_r u + r_u\) and \(-q^e_w c_w\) on \(Q_1\).
If we apply Step 2, then $Q_1$ will become

$$Q_2 = \begin{pmatrix}
Q' & O_{s+1,2} & O_{s+1,r} \\
O_{2,s+r} & 1 & 0 \\
O_r & 0 & 1 - q^2 \\
O_{r.s+r} & (Q'')^r & qD_2
\end{pmatrix}.$$

Note that $Q_2(x_1 \cdots x_s y_1 \cdots y_t u v)$ can be obtained by performing Steps 1 and 2 to $qD_H$. Thus $1$ and $1 - q^2$ are pre-invariant factors of $H$. We convert $Q'$ to the Smith normal form. By Corollary 2.3, all the entries of the resulting $Q'$ are divisible by $1 - q^2$. Then $[1, 1 - q^2] \subseteq \text{Inv}(H)$. Thus the invariant factors of $Q'$ is $\text{Inv}(H) \setminus [1, 1 - q^2]$. Since $Q_2 = Q_2[u w z_1 \cdots z_r]$ is equivalent to $qD_K$, we obtain $\text{Inv}(K)$ from $Q_2$. Therefore, $\text{Inv}(K) \cup \text{Inv}(H) \setminus [1, 1 - q^2]$ is a pre-invariant factor set of $G$.

By a similar proof of Theorem 4.1 we have

**Theorem 4.2.** Let $H$ and $K$ be two subgraphs of $G$ such that $G = H \cup K$ and $H$ and $K$ have one vertex in common. Then $\text{Inv}(K) \cup \text{Inv}(H) \setminus [1]$ is a pre-invariant factor set of $G$.

**Corollary 4.3.** Let $G$ be a bipartite graph. Suppose $v \in V(G)$ of degree 1. Then $\text{Inv}(G) = \text{Inv}(G - v) \cup [1 - q^2]$.

**Proof.** Let $u$ be the vertex adjacent to $v$. Let $H$ be the path $uv$ and $K = G - v$. They are bipartite. Thus $\text{Inv}(H) = [1, 1 - q^2]$ and $\text{Inv}(K) = [1, 1 - q^2, \ldots]$. By Theorem 4.2, Corollary 2.3 and since $1 - q^2$ is an invariant factor of $G$, the corollary follows.

By using Corollary 4.3, one can easily compute the invariant factors of tree with $n$ vertices is $[1, (1 - q^2)[n - 1]$ times].

The following theorem is a generalization of Theorem 4.1.

**Theorem 4.4.** Let $H$ and $K$ be two subgraphs of $G$ such that $G = H \cup K$ and $H \cap K$ is connected. Let $\text{Inv}(H \cap K) = \{f_1, f_2, \ldots, f_t\}$. If $\text{Inv}(H \cap K)$ is the first $t$ invariant factors of $H$ and for any $x \in V(H)$ there exists $y \in V(H \cap K)$ such that for any $z \in V(K)$, $d(x, z) = d(x, y) + d(y, z)$, then $\text{Inv}(K) \cup \text{Inv}(H) \setminus \text{Inv}(H \cap K)$ is a pre-invariant factor set of $G$.

**Proof.** Let $Y = V(H \cap K)$, $X = V(H) \setminus Y$ and $Z = V(K) \setminus Y$. We arrange the vertices in the following order: Vertices of $X$ first, $Y$ second and $Z$ last. Then the $Q_G$ is formed as

$$Q_G = \begin{pmatrix}
Q_X & O_{XY} & O_{XZ} \\
O_{XY} & Q_Y & O_{YZ} \\
O_{XZ} & O_{YZ} & Q_Z
\end{pmatrix},$$

where all block matrices are of their corresponding sizes. By the hypothesis, for each $x \in X$ there exists $y \in Y$ such that $d(x, z) = d(x, y) + d(y, z)$ for all $z \in Y \cup Z$. We apply the row operation $-q^{d(x,y)}r_y + r_x$ and the column operation $-q^{d(x,y)}c_y + c_x$ for each $x \in X$. Then $Q$ becomes

$$Q_1 = \begin{pmatrix}
Q_X' & O & O \\
O & Q_Y & O_{YZ} \\
O & O & Q_Z
\end{pmatrix}. $$

Since $\text{Inv}(H \cap K) = \{f_2, \ldots, f_t\}$, there exist two invertible matrices $P, P'$ such that $PQYP' = \text{diag}(1, f_2, \ldots, f_t) = Q_Y'$. Then

$$\begin{pmatrix}I_{|X|} & O & O \\
O & P & O \\
O & O & I_{|Z|}
\end{pmatrix}Q_1 \begin{pmatrix}I_{|X|} & O & O \\
O & P' & O \\
O & O & I_{|Z|}
\end{pmatrix} = \begin{pmatrix}Q_X & O & O \\
O & Q_Y' & P Q_{YZ} \\
O & P' Q_{YZ} & Q_Z
\end{pmatrix}. $$

(4.1)

Since $\text{Inv}(H \cap K)$ is the first $t$ invariant factors of $H$, similar to the proof of Theorem 4.1 the assertion holds.

**Theorem 4.5.** Let $H$ and $K$ be two subgraphs of $G$ such that $G = H \cup K$ and $H \cap K$ is connected. If $\text{Inv}(H \cap K) \subseteq \text{Inv}(H) \cap \text{Inv}(K)$ and for any $x \in V(H)$ there exists $y \in V(H \cap K)$ such that for any $z \in V(K)$, $d(x, z) = d(x, y) + d(y, z)$, then $\text{Inv}(K) \cup \text{Inv}(H) \setminus \text{Inv}(H \cap K)$ is a pre-invariant factor set of $G$. 
Proof. By the same proof of Theorem 4.4, we have the matrix described in (4.1). We convert the matrix \((Q'_Y P Q'_YZ Q_Z)\) to Smith normal form \(S_\mathcal{K}\). Since \(\text{Inv}(H \cap K) \subseteq \text{Inv}(K)\), 1, \(f_2, \ldots, f_t\) are elements of the diagonal of \(S_\mathcal{K}\). By suitably exchanging rows and columns, we can move 1, \(f_2, \ldots, f_t\) to the first \(t\) elements of the diagonal of \(S_\mathcal{K}\). That is, the matrix in (4.1) becomes \((Q'_X O Q'_Y O Q'_Z)\), where \(Q'_Z\) is a diagonal matrix. Convert the matrix \((Q'_X O Q'_Y)\) to Smith normal form \(S_\mathcal{H}\). Since \(\text{Inv}(H \cap K) \subseteq \text{Inv}(H)\), 1, \(f_2, \ldots, f_t\) also are elements of the diagonal of \(S_\mathcal{H}\). Thus \(\text{Inv}(K) \cup \text{Inv}(H) \setminus \text{Inv}(H \cap K)\) is a pre-invariant factor set of \(G\). \(\square\)

A polyomino is a graph obtained from the grid \(P_m \times P_n\) by deleting some squares and all the bounded faces are 4-faces. Fig. 3 shows a polyomino. By using Theorem 4.4, one can compute the invariant factors of any polyomino. We leave it to the reader as an exercise.

5. Computation results of some bipartite graphs (2)

In this section we will compute some bipartite graphs, for example the hexagonal trees, which is a class of well-known molecular graphs.

A graph \(G\) is called a polygonal tree if it consists of finitely many regular polygons (we assume any two distinct polygons are not coplanar) and has the following two properties:

1. Any two distinct polygons are disjoint or have exactly one edge in common (such edge can be a common edge of several polygons).
2. The diagram obtained by joining the centroids of the polygons to the mid-point of the common edge has no closed curve.

If all polygons of a polygonal tree \(G\) are the same, say \(s\)-gons, then \(G\) is called a \(s\)-gonal tree. 6-gonal tree is called hexagonal tree. Consider the diagram defined in the condition 2. If we let the centroids and the mid-points of common edges of some polygons as “red” vertices and “green” vertices, respectively, and the straight line segments as edges of a bipartite graph. Then this graph is a tree.

Example 5.1. Let \(G\) be the graph described in Fig. 4. Let \(H = G[a, b, c, d, i, j]\) the induced subgraph of \(G\). By Theorems 3.5 and 4.1 we have

\[
\text{Inv}(H) = \{1, 1 - q^2, 1 - q^2, 1 - q^2, (1 - q^2)^2, (1 - q^2)^2\}.
\]

By Theorems 3.5 and 4.1 again, a pre-invariant factor set of \(G\) is

\[
\{1 - q^2, 1 - q^2, (1 - q^2)^2\} \cup \{1, 1 - q^2, 1 - q^2, 1 - q^2, (1 - q^2)^2, (1 - q^2)(1 - q^6)\}.
\]

By Corollary 2.6, \(\text{Inv}(G) = \{1, 1 - q^2 [5 \text{ times}], (1 - q^2)^2 [\text{thrice}], (1 - q^2)(1 - q^6)\}.

In general, we have the following theorem.
Theorem 5.1. Suppose \( G \) is a polygonal tree consisting of \( C_{2s_1}, C_{2s_2}, \ldots, C_{2s_n} \). Let \( r_1 > r_2 > \cdots > r_t \geq 2 \) be distinct values of \( s_1, s_2, \ldots, s_n \) with multiplicities \( n_1, n_2, \ldots, n_t \), respectively. Then the invariant factors of \( G \) are

\[
1 \text{ [once]},
\]

\[
1 - q^2 \left[ n_1 r_1 + \cdots + n_t r_t - n + 1 = s_1 + \cdots + s_n - n + 1 \text{ times}\right],
\]

\[
(1 - q^2)^2 [n_2 r_2 + \cdots + n_t r_t - n + 2n_1 \text{ times}],
\]

\[
(1 - q^2)^2 \left( \frac{1 - q^{2r_1}}{1 - q^2} \right) [n_1 (r_1 - 2) - n_2 (r_2 - 2) \text{ times}],
\]

\[
\vdots
\]

\[
(1 - q^2)^2 \left( \frac{1 - q^{2r_1}}{1 - q^2} \right) \left( \frac{1 - q^{2r_2}}{1 - q^2} \right) \cdots \left( \frac{1 - q^{2r_t-1}}{1 - q^2} \right) [n_{t-1} (r_{t-1} - 2) - n_t (r_t - 2) \text{ times}],
\]

\[
(1 - q^2)^2 \left( \frac{1 - q^{2r_1}}{1 - q^2} \right) \left( \frac{1 - q^{2r_2}}{1 - q^2} \right) \cdots \left( \frac{1 - q^{2r_t}}{1 - q^2} \right) [n_t (r_t - 2) \text{ times}].
\]

Proof. Let \( T \) be the tree described in the condition 2. Each red vertex represents a polygon. Choose a red leaf of \( T \), apply Theorems 4.1 and 3.5 and remove it. Repeat this process until all red leaves are removed. Then remove all green leaves. Repeat the process until all vertices are removed. By Corollary 2.6, the theorem follows. \( \square \)

Thus we have many non-isomorphic graphs whose invariant factors are the same.

Corollary 5.2. The invariant factors of a \( 2s \)-gonal tree consisting of \( n \) \( 2s \)-cycles are

\[
1 \text{ [once]},
\]

\[
1 - q^2 \left[ sn - n + 1 \text{ times}\right],
\]

\[
(1 - q^2)^2 [n \text{ times}],
\]

\[
(1 - q^2)^2 (1 - q^{2s}) [(s - 2)n \text{ times}].
\]

Example 5.2. The invariant factors of a hexagonal tree with \( n \) hexagons is

\[
\begin{align*}
& \underbrace{2n+1 \text{ times}}_{1}, \underbrace{\cdots, 1 - q^2, 1 - q^2, \cdots, 1 - q^2}_{n \text{ times}}, \underbrace{(1 - q^2)^2, (1 - q^2)^2, \cdots, (1 - q^2)^2}_{n \text{ times}}, \\
& \cdots, \underbrace{(1 - q^2)^2(1 - q^6), \cdots, (1 - q^2)^2(1 - q^6)}_{n \text{ times}}.
\end{align*}
\]

One can compute some pericondensed benzenoid molecular system graphs by using Theorem 4.4. For example, hexagonal nets, hexagonal parallelisums etc., which were defined in [9–14].
6. Computation results of some non-bipartite graphs

6.1. Complete graphs

The distance matrix of \( K_3 \) is a right cyclic matrix whose first row is \((0, 1, 1, \ldots, 1)\). Similar to Section 3.2, we obtain the spectrum of \( Q_{K_3} \) is \( \{ f(q, \zeta^k) \mid 0 \leq k \leq s \leq 1 \} \) where \( f(q, \lambda) = 1 + q \sum_{j=1}^{s-1} \lambda^j \) and \( \zeta \) is a primitive \( s \)th root of 1. It is easy to compute that the eigenvalues are \( 1 + (s - 1)q, 1 - q \) \([s - 1]\) times. Thus the invariant factors of \( K_3 \) are \( 1, 1 - q, 1 - q \) \([s - 2]\) times and \((1 - q)(1 + (s - 1)q)\).

6.2. Odd cycles

From (3.1) a set of pre-invariant factors of \( C_{2s+1} \circ N_n \) is

\[
g_{s,n}(q, \zeta^k) = 1 - q^2, \quad k \not\equiv 0(\text{mod } n)
\]

and

\[
g_{s,n}(q, \zeta^{nk}) = 1 + (n - 1)q^2 + n \sum_{i=1}^{s} (\zeta^{ni} + \zeta^{-ni})q^i, \quad 0 \leq k \leq 2s,
\]

where \( \zeta \) is a \((2s + 1)\)th primitive root of 1.

Consider the \((2s + 1)\) cycle, i.e., when \( n = 1 \), a set of pre-invariant factors of \( C_{2s+1} \) is

\[
f_{2s+1}(q, \zeta^k) = g_{s,1}(q, \zeta^k) = 1 + \sum_{i=1}^{s} (\zeta^{ki} + \zeta^{-ki})q^i, \quad 0 \leq k \leq 2s.
\]

They seem difficult to be factorized in general. Let us consider two special cases.

**Example 6.1.** A set of pre-invariant factors of \( C_3 \) is \( f_3(q, 1) = 1 + 2q, f_3(q, \omega) = 1 - q = f_3(q, \omega^2) \), where \( \omega \) is a primitive root of \( x^3 = 1 \). Thus the invariant factors of \( C_3 \) are \( 1, 1 - q, 1 - q \) \((1 - q)(1 + 2q)\).

**Example 6.2.** A set of pre-invariant factors of \( C_5 \) is \( f_5(q, 1) = 1 + 2q + 2q^2, f_5(q, \zeta^5) = f_5(q, \zeta^4) = 1 + (\zeta + \zeta^{-1})q + (\zeta^2 + \zeta^{-2})q^2 = (1 - q)(1 - (\zeta^2 + \zeta^{-2})q), f_5(q, \zeta^2) = f_5(q, \zeta^3) = (1 - q)(1 - (\zeta + \zeta^{-1})q) \), where \( \zeta \) is a primitive root of \( x^5 = 1 \). Thus the invariant factors of \( C_5 \) are \( 1, 1 - q, 1 - q, 1 - q(1 + q - q^2), 1 - q(1 + q - q^2)(1 + 2q + 2q^2) \).

6.3. Miscellaneous

**Example 6.3.** Consider \( C_{2s} \circ K_n \). Similar to Section 3.2, a set of pre-invariant factors of \( C_{2s} \circ K_n \) is \( f(q, \zeta^k) = 1 - q^2, k \not\equiv 0(\text{mod } n) \); and \( f(q, \zeta^{nk}) = 1 + (n - 1)q + (1 - k^2)q^2 + n \sum_{i=1}^{s-1} (\zeta^{ni} + \zeta^{-ni})q^i, 0 \leq k \leq 2s - 1 \), where \( \zeta \) is a primitive \( 2s \)th root of 1.

For \( n = 2 \) and \( s = 2 \). A set of pre-invariant factors of \( C_4 \circ K_2 \) (Fig. 5a) is \( f(q, 1) = 1 + 5q + 2q^2, f(q, \zeta) = f(q, \zeta^3) = f(q, \zeta^{5}) = f(q, \zeta^{7}) = 1 - q^2, f(q, \zeta^{3}) = (1 - q)(1 + 2q) = f(q, \zeta^5), f(q, \zeta^{7}) = (1 - q)(1 - 2q) \). Thus the invariant factors of \( C_4 \circ K_2 \) are \( 1, 1 - q, 1 - q, 1 - q, 1 - q^2, 1 - q^2, (1 - q^2)(1 + 2q), (1 - q^2)(1 - 4q^2)(1 + 5q + 2q^2) \).

**Example 6.4.** Consider the graph \( G \) described in Fig. 5b. By Theorem 3.5 and Example 6.1 we have Inv\((C_4) = \{1, 1 - q^2, 1 - q^2, (1 - q^2)^2\} \) and Inv\((C_3) = \{1, 1 - q, (1 - q)(1 + 2q)\} \). Applying Theorem 4.1, a pre-invariant factor set of \( G \) is
Thus the invariant factors are pre-invariant factor set of $G$

Example 6.5. Consider the graph $G$ described in Fig. 5c. Applying Theorem 4.2 and the results of Examples 6.1 and 6.2, a pre-invariant factor set of $G$ is

$$\{1, 1 - q, (1 - q)(1 + 2q), 1 - q, (1 - q)(1 + q - q^2), 1 - q(1 + q - q^2)(1 + 2q + 2q^2)\}.$$ 

Thus the invariant factors are

$$1, 1 - q, 1 - q, 1 - q, (1 - q)(1 + q - q^2), (1 - q)(1 + q - q^2)(1 + 2q)(1 + 2q).$$

Finally, we consider the first example (Example 2.1) again.

Example 6.6. Consider the graph $G$ in Example 2.1. Let $H = G[R_1, R_2, R_3, R_7] \cong C_4$ and $K = G\{R_2\} \cong P_2 \times P_3$. Then $H \cap K \cong P_3$. From Example 5.1,

$$\text{Inv}(K) = \{1, 1 - q^2, 1 - q^2, 1 - q^2, (1 - q^2)^2, (1 - q^2)^2\}.$$ 

By Theorem 4.4 and Corollary 2.6,

$$\text{Inv}(G) = \{1, 1 - q^2, 1 - q^2, 1 - q^2, (1 - q^2)^2, (1 - q^2)^2\}.$$ 

7. Conclusion

This paper has presented some methods to find the invariant factors of graphs. This is the initial work on the problem. Invariant factors of some graphs derived from hyperplane arrangements have not been found yet, for example the Cayley graph described in Example 2.3. Recently, the invariant factors of Cartesian product of graphs have been discussed. The invariant factors of some graphs derived from hyperplane arrangements have not been found yet, for example the Cayley graph described in Fig. 5c.

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References