Graph isomorphism and graphs identified by multivariate spectrum

Abstract

1 Introduction

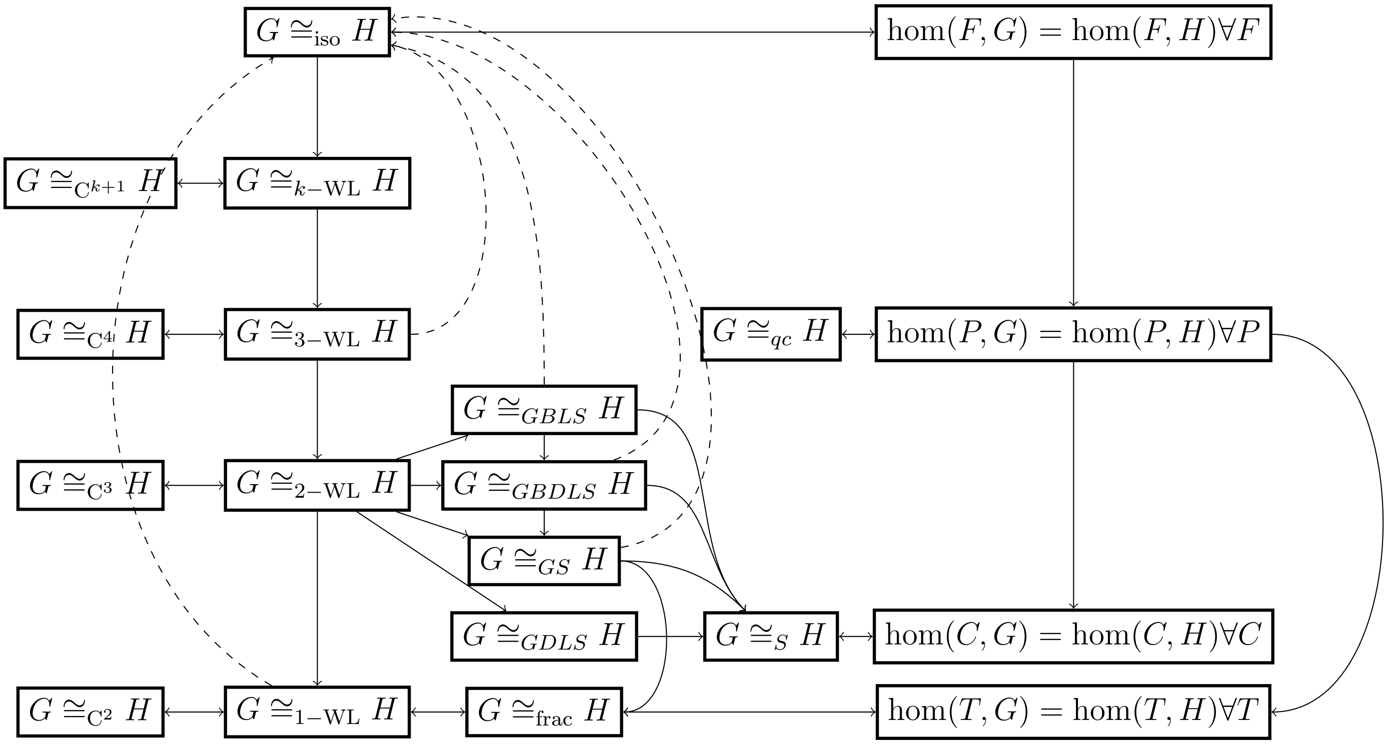

Figure 1: Relation among equivalence classes of graphs

2 Preliminary

Let $\boldsymbol{A} = (A_1, A_2, \ldots, A_k)$ be a k-tuple of $n \times n$ integral matrices. Let $\boldsymbol{s} = (s_1, s_2, \ldots, s_k)$ be a k-tuple of complex variables. We define

$$W_{\boldsymbol{A}}(\boldsymbol{s}) = W_{A_1,A_2,\ldots,A_k}(s_1, s_2, \ldots, s_k) = \sum_{i=1}^{k} s_i A_i. \tag{1}$$

Denote by $\phi_{\boldsymbol{A}}(\boldsymbol{s}; t) = \det(tI - W_{\boldsymbol{A}}(\boldsymbol{s}))$ the characteristic polynomial of $W_{\boldsymbol{A}}(\boldsymbol{s})$.

Theorem 2.1. *Let $\boldsymbol{A} = (A_1, A_2, \ldots, A_k)$ be a k-tuple of $n \times n$ integral matrices. Let $\boldsymbol{s} = (s_1, s_2, \ldots, s_k)$ be a k-tuple of complex variables. Then there exist values $\boldsymbol{s}_0 = (\hat{s}_1, \hat{s}_2, \ldots, \hat{s}_k)$ such that $\phi_{\boldsymbol{A}}(\boldsymbol{s}; t)$ and $\phi_{\boldsymbol{B}}(\boldsymbol{s}; t)$ are identically the same in t if and only if $\phi_{\boldsymbol{A}}(\boldsymbol{s}_0; t) = \phi_{\boldsymbol{B}}(\boldsymbol{s}_0; t)$.*

Proof. Let $\phi_{\boldsymbol{A}}(\boldsymbol{s}; t) = \sum_{i=0}^{n} c_{\boldsymbol{A}}^{(i)}(\boldsymbol{s}) t^i$ be the expansion of $\phi_{\boldsymbol{A}}(\boldsymbol{s}; t)$. Let $\phi_{\boldsymbol{B}}(\boldsymbol{s}; t) = \sum_{i=0}^{n} c_{\boldsymbol{B}}^{(i)}(\boldsymbol{s}) t^i$ be the expansion of $\phi_{\boldsymbol{B}}(\boldsymbol{s}; t)$. Then $\phi_{\boldsymbol{A}}(\boldsymbol{s}; t)$ and $\phi_{\boldsymbol{B}}(\boldsymbol{s}; t)$ are not identical if and only if there exists an index i such that the multivariate polynomial

$$d_i(\boldsymbol{s}) = c_{\boldsymbol{A}}^{(i)}(\boldsymbol{s}) - c_{\boldsymbol{B}}^{(i)}(\boldsymbol{s}) \tag{2}$$

is not identically zero. Take k algebraically independent numbers $\boldsymbol{s}_0 = (\hat{s}_1, \hat{s}_2, \ldots, \hat{s}_k)$ over $\mathbb{Z}$ suffice. $\square$

Theorem 2.2. *Let A_1 and B_1 be two real symmetric matrices of order n. Let e_i, $i = 1, 2, \ldots, p$ be zero-one vectors of length n such that the positions of the ones are disjoint. Let $J_{i,j} = e_i e_j^\top$ for $i, j = 1, 2, \ldots, p$ and $k = 1 + p^2$. Let $\boldsymbol{A} = (A_1, A_2, \ldots, A_k) = (A_1, J_{1,1}, J_{1,2}, \ldots, J_{p,p})$ and $\boldsymbol{B} = (B_1, B_2, \ldots, B_k) = (B_1, J_{1,1}, J_{1,2}, \ldots, J_{p,p})$. Then the matrices $W_{\boldsymbol{A}}(\boldsymbol{s})$ and $W_{\boldsymbol{B}}(\boldsymbol{s})$ have identically the same characteristic polynomials if and only if they are similar via a fixed orthogonal matrix Q, independent of $\boldsymbol{s}$, such that*

1. *Q is a block matrix with blocks corresponding to the ones in $e_i, i = 2, 3, \ldots, k$;*
2. *the sum of each row or column of Q is 1.*

Moreover, $Q^\top \widetilde{W}_{A_1} = \widetilde{W}_{B_1}$, where

$$\widetilde{W}_A = [e_1, Ae_1, \ldots, A^{n-1}e_1, e_2, Ae_2, \ldots, A^{n-1}e_2, \ldots, e_p, Ae_p, \ldots, A^{n-1}e_p]. \tag{3}$$

Proof. Note that $J_{i,j}, i, j = 1, 2, \ldots, p$ commute with each other. So there exists an orthogonal matrix O such that

$$O^\top J_{i,j} O = n_{i,j} E_{i,j}, \tag{4}$$

where $E_{i,j}$ is the matrix whose only nonzero entry is a 1 in the (i,j)-entry. Replace $\hat{A}_i = O^\top A_i O$, $\hat{B}_i = O^\top B_i O$, for $i = 1, 2, \ldots, k$. For $\hat{\boldsymbol{A}} = (\hat{A}_1, \hat{A}_2, \ldots, \hat{A}_k)$ and $\hat{\boldsymbol{B}} = (\hat{B}_1, \hat{B}_2, \ldots, \hat{B}_k)$, we have

$$\det(tI - x\hat{A}_1 - \sum_{i,j=1}^{p} s_{i,j} n_{i,j} E_{i,j}) = \det(tI - x\hat{B}_1 - \sum_{i,j=1}^{p} s_{i,j} n_{i,j} E_{i,j}) \tag{5}$$

for all $x, s_{1,1}, s_{1,2}, \ldots, s_{p,p} \in \mathbb{C}$. By expanding the minors along the first p rows, we get

$$\begin{aligned} &\sum_{\substack{K,L \subseteq F \\ |K|=|L|}} \sum_{\sigma: K \leftrightarrow L} (-1)^{|K|} \left(\prod_{i \in K} s_{i,\sigma(i)} n_{i,\sigma(i)} \right) \det(tI - x\hat{A}_1)_{[K],[L]} \\ = &\sum_{\substack{K,L \subseteq F \\ |K|=|L|}} \sum_{\sigma: K \leftrightarrow L} (-1)^{|K|} \left(\prod_{i \in K} s_{i,\sigma(i)} n_{i,\sigma(i)} \right) \det(tI - x\hat{B}_1)_{[K],[L]} \end{aligned}$$

where F denotes the set $\{1, 2, \ldots, p\}$ and $X_{[K],[L]}$ denotes the submatrix of X obtained by deleting the rows corresponding to K and the columns corresponding to L. Since $s_{i,j}$, $1 \leq i, j \leq p$ are arbitrary, we get

$$\det(tI - x\hat{A}_1)_{[K],[L]} = \det(tI - x\hat{B}_1)_{[K],[L]}, \tag{6}$$

for $K, L \subseteq F$ with $|K| = |L|$. It follows that $(\hat{A}_1)_{[F],[F]}$ and $(\hat{B}_1)_{[F],[F]}$ are orthogonally similar. We may assume that after suitable similarities of the form $P = \begin{bmatrix} I_p & 0 \\ 0 & U \end{bmatrix}$ it holds

$$\hat{A}_1 = \begin{bmatrix} a_{1,1} & \cdots & a_{1,p} & \alpha_{p+1,1}^\top & \cdots & \alpha_{q,1}^\top \\ \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ a_{p,1} & \cdots & a_{p,p} & \alpha_{p+1,p}^\top & \cdots & \alpha_{q,k}^\top \\ \alpha_{p+1,1} & \cdots & \alpha_{p+1,p} & \lambda_{p+1} I_{m_{p+1}} & 0 & 0 \\ \vdots & \vdots & \vdots & 0 & \ddots & 0 \\ \alpha_{q,1} & \cdots & \alpha_{q,p} & 0 & 0 & \lambda_q I_{m_q} \end{bmatrix} \tag{7}$$

and

$$\hat{B}_1 = \begin{bmatrix} b_{1,1} & \cdots & b_{1,p} & \beta_{p+1,1}^\top & \cdots & \beta_{q,1}^\top \\ \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ b_{p,1} & \cdots & b_{p,p} & \beta_{p+1,p}^\top & \cdots & \beta_{q,k}^\top \\ \beta_{p+1,1} & \cdots & \beta_{p+1,p} & \lambda_{p+1} I_{m_{p+1}} & 0 & 0 \\ \vdots & \vdots & \vdots & 0 & \ddots & 0 \\ \beta_{q,1} & \cdots & \beta_{q,p} & 0 & 0 & \lambda_q I_{m_q} \end{bmatrix}, \tag{8}$$

where $\lambda_{p+1}, \dots, \lambda_q$ are the distinct eigenvalues of $\hat{A}_{[F],[F]}$ (and also of $\hat{B}_{[F],[F]}$). For $i, \ell \in F$, we define

$$\mathfrak{A}_{i,\ell} = \delta_{i,\ell} t - x a_{i,\ell} - s_{i,\ell} n_{i,\ell} + \sum_{j=p+1}^{q} \frac{x^2 \langle \alpha_{j,i}, \alpha_{j,\ell} \rangle}{t - x\lambda_j}, \tag{9}$$

and

$$\mathfrak{B}_{i,\ell} = \delta_{i,\ell} t - x b_{i,\ell} - s_{i,\ell} n_{i,\ell} + \sum_{j=p+1}^{q} \frac{x^2 \langle \beta_{j,i}, \beta_{j,\ell} \rangle}{t - x\lambda_j}, \tag{10}$$

where $\delta_{i,\ell}$ is the Kronecker delta function, namely

$$\delta_{i,\ell} = \begin{cases} 1, & i = \ell, \\ 0, & i \neq \ell. \end{cases} \tag{11}$$

Expand Eq. (6) with $K = L = \{2, 3, \dots, p\}$, and we get

$$\det(tI - x\hat{A}_1)_{[\{2,3,\dots,p\}],[\{2,3,\dots,p\}]} = \mathfrak{A}_{1,1} \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j} \tag{12}$$

and

$$\det(tI - s_1\hat{B}_1)_{[\{2,3,\dots,p\}],[\{2,3,\dots,p\}]} = \mathfrak{B}_{1,1} \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j}. \tag{13}$$

We conclude that $a_{1,1} = b_{1,1}$ and $\langle \alpha_{j,1}, \alpha_{j,1} \rangle = \langle \beta_{j,1}, \beta_{j,1} \rangle$ for $j = p, p+1, \dots, q$. Similarly, we have $a_{i,i} = b_{i,i}$ and $\langle \alpha_{j,i}, \alpha_{j,i} \rangle = \langle \beta_{j,i}, \beta_{j,i} \rangle$ for $i = 1, 2, \dots, p$ and $j = p, p+1, \dots, q$. Now we expand Eq. (6) with $K = L = \{3, 4, \dots, p\}$ and get

$$\det(tI - x\hat{A}_1)_{[\{3,4,\dots,p\}],[\{3,4,\dots,p\}]} = (\mathfrak{A}_{1,1}\mathfrak{A}_{2,2} - \mathfrak{A}_{1,2}\mathfrak{A}_{2,1}) \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j}, \tag{14}$$

and

$$\det(tI - x\hat{B}_1)_{[\{3,4,\dots,p\}],[\{3,4,\dots,p\}]} = (\mathfrak{B}_{1,1}\mathfrak{B}_{2,2} - \mathfrak{B}_{1,2}\mathfrak{B}_{2,1}) \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j}. \tag{15}$$

Therefore,

$$\mathfrak{A}_{1,1}\mathfrak{A}_{2,2} - \mathfrak{A}_{1,2}\mathfrak{A}_{2,1} = \mathfrak{B}_{1,1}\mathfrak{B}_{2,2} - \mathfrak{B}_{1,2}\mathfrak{B}_{2,1}. \tag{16}$$

Consider the polynomial term, and we get

$$\begin{aligned} &(t - xa_{11} - s_{11}n_{11})(t - xa_{22} - s_{22}n_{22}) - (-xa_{12} - s_{12}n_{12})(-xa_{21} - s_{21}n_{21}) && (17) \\ =&(t - xb_{11} - s_{11}n_{11})(t - xb_{22} - s_{22}n_{22}) - (-xb_{12} - s_{12}n_{12})(-xb_{21} - s_{21}n_{21}). && (18) \end{aligned}$$

Hence, $a_{1,2} = b_{1,2}$ and $a_{2,1} = b_{2,1}$. Similarly, we have $a_{i,j} = b_{i,j}$ for $1 \leq i, j \leq p$. Consider the coefficient of $\frac{1}{t - x\lambda_j}$, and we get

$$\begin{aligned}
&(t - xa_{11} - s_{11}n_{11})(x^2\langle\alpha_{j2}, \alpha_{j2}\rangle) + (t - xa_{22} - s_{22}n_{22})(x^2\langle\alpha_{j1}, \alpha_{j1}\rangle) && (19)\\
&- (-xa_{12} - s_{12}n_{12})(x^2\langle\alpha_{j2}, \alpha_{j1}\rangle) - (-xa_{21} - s_{21}n_{21})(x^2\langle\alpha_{j1}, \alpha_{j2}\rangle) && (20)\\
=&(t - xb_{11} - s_{11}n_{11})(x^2\langle\beta_{j2}, \beta_{j2}\rangle) + (t - xb_{22} - s_{22}n_{22})(x^2\langle\beta_{j1}, \beta_{j1}\rangle) && (21)\\
&- (-xb_{12} - s_{12}n_{12})(x^2\langle\beta_{j2}, \beta_{j1}\rangle) - (-xb_{21} - s_{21}n_{21})(x^2\langle\beta_{j1}, \beta_{j2}\rangle). && (22)
\end{aligned}$$

Hence, $\langle\alpha_{j1}, \alpha_{j2}\rangle = \langle\beta_{j1}, \beta_{j2}\rangle$, $\langle\alpha_{j2}, \alpha_{j1}\rangle = \langle\beta_{j2}, \beta_{j1}\rangle$ for $j = p+1, p+2, \ldots, q$. Similarly, we have $\langle\alpha_{j,i}, \alpha_{j,\ell}\rangle = \langle\beta_{j,i}, \beta_{j,\ell}\rangle$, for $j = p+1, p+2, \ldots, q$, $1 \leq i \neq \ell \leq p$. Therefore, there exists an orthogonal matrix $R = \begin{bmatrix} I_p & 0 \\ 0 & V \end{bmatrix}$ such that $\hat{A}_1 = R^\top \hat{B}_1 R$. Consider $Q = OR$, then $Q^\top W_{\boldsymbol{A}}(\boldsymbol{s})Q = W_{\boldsymbol{B}}(\boldsymbol{s})$, and it satisfies the conditions in the theorem. □

Theorem 2.3. *Let A_1 and B_1 be two real symmetric matrices of order n. Let e_i, $i = 1, 2, \ldots, p$ be zero-one vectors of length n such that the positions of the ones are disjoint. Let $J_{i,i} = e_i e_i^\top$ for $i, j = 1, 2, \ldots, p$ and $k = 1 + p$. Let $\boldsymbol{A} = (A_1, A_2, \ldots, A_k) = (A_1, J_{1,1}, J_{2,2}, \ldots, J_{p,p})$ and $\boldsymbol{B} = (B_1, B_2, \ldots, B_k) = (B_1, J_{1,1}, J_{2,2}, \ldots, J_{p,p})$. Suppose $e_i^\top A_1 e_j \neq 0$ for $1 \leq i \neq j \leq p$ or $p \leq 2$. Then the matrices $W_{\boldsymbol{A}}(\boldsymbol{s})$ and $W_{\boldsymbol{B}}(\boldsymbol{s})$ have identically the same characteristic polynomials if and only if they are similar via a fixed orthogonal matrix Q, independent of $\boldsymbol{s}$, such that*

1. *Q is a block matrix with blocks corresponding to the ones in $e_i, i = 2, 3, \ldots, k$;*
2. *the sum of each row or column of Q is 1.*

Moreover, $Q^\top \widetilde{W}_{A_1} = \widetilde{W}_{B_1}$, where

$$\widetilde{W}_A = [e_1, Ae_1, \ldots, A^{n-1}e_1, e_2, Ae_2, \ldots, A^{n-1}e_2, \ldots, e_p, Ae_p, \ldots, A^{n-1}e_p]. \tag{23}$$

Proof. Note that $J_{i,i}, i = 1, 2, \ldots, p$ commute with each other. So there exists an orthogonal matrix O such that

$$O^\top J_{i,i} O = n_{i,i} E_{i,i}, \tag{24}$$

where $E_{i,j}$ is the matrix whose only nonzero entry is a 1 in the (i, j)-entry. Replace $\hat{A}_i = O^\top A_i O$, $\hat{B}_i = O^\top B_i O$, for $i = 1, 2, \ldots, k$. For $\hat{\boldsymbol{A}} = (\hat{A}_1, \hat{A}_2, \ldots, \hat{A}_k)$ and $\hat{\boldsymbol{B}} = (\hat{B}_1, \hat{B}_2, \ldots, \hat{B}_k)$, we have

$$\det(tI - x\hat{A}_1 - \sum_{i=1}^{p} s_{i,i} n_{i,i} E_{i,i}) = \det(tI - x\hat{B}_1 - \sum_{i=1}^{p} s_{i,i} n_{i,i} E_{i,i}) \tag{25}$$

for all $x, s_{1,1}, s_{1,2}, \ldots, s_{p,p} \in \mathbb{C}$. By expanding the minors along the first p rows, we get

$$\begin{aligned}&\sum_{K \subseteq F} (-1)^{|K|} \left(\prod_{i \in K} s_{i,i} n_{i,i} \right) \det(tI - x\hat{A}_1)_{[K],[K]} \\ = &\sum_{K \subseteq F} (-1)^{|K|} \left(\prod_{i \in K} s_{i,i} n_{i,i} \right) \det(tI - x\hat{B}_1)_{[K],[K]}\end{aligned}$$

where F denotes the set $\{1, 2, \ldots, p\}$ and $X_{[K],[L]}$ denotes the submatrix of X obtained by deleting the rows corresponding to K and the columns corresponding to L. Since $s_{i,i}$, $1 \leq i \leq p$ are arbitrary, we get

$$\det(tI - x\hat{A}_1)_{[K],[K]} = \det(tI - x\hat{B}_1)_{[K],[K]}, \tag{26}$$

for $K \subseteq F$. It follows that $(\hat{A}_1)_{[F],[F]}$ and $(\hat{B}_1)_{[F],[F]}$ are orthogonally similar. We may assume that after suitable similarities of the form $P = \begin{bmatrix} I_p & 0 \\ 0 & U \end{bmatrix}$ it holds

$$\hat{A}_1 = \begin{bmatrix} a_{1,1} & \cdots & a_{1,p} & \alpha_{p+1,1}^\top & \cdots & \alpha_{q,1}^\top \\ \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ a_{p,1} & \cdots & a_{p,p} & \alpha_{p+1,p}^\top & \cdots & \alpha_{q,k}^\top \\ \alpha_{p+1,1} & \cdots & \alpha_{p+1,p} & \lambda_{p+1} I_{m_{p+1}} & 0 & 0 \\ \vdots & \vdots & \vdots & 0 & \ddots & 0 \\ \alpha_{q,1} & \cdots & \alpha_{q,p} & 0 & 0 & \lambda_q I_{m_q} \end{bmatrix} \tag{27}$$

and

$$\hat{B}_1 = \begin{bmatrix} b_{1,1} & \cdots & b_{1,p} & \beta_{p+1,1}^\top & \cdots & \beta_{q,1}^\top \\ \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ b_{p,1} & \cdots & b_{p,p} & \beta_{p+1,p}^\top & \cdots & \beta_{q,k}^\top \\ \beta_{p+1,1} & \cdots & \beta_{p+1,p} & \lambda_{p+1} I_{m_{p+1}} & 0 & 0 \\ \vdots & \vdots & \vdots & 0 & \ddots & 0 \\ \beta_{q,1} & \cdots & \beta_{q,p} & 0 & 0 & \lambda_q I_{m_q} \end{bmatrix}, \tag{28}$$

where $\lambda_{p+1}, \ldots, \lambda_q$ are the distinct eigenvalues of $\hat{A}_{[F],[F]}$ (and also of $\hat{B}_{[F],[F]}$). For $i, \ell \in F$, we define

$$\mathfrak{A}_{i,\ell} = \delta_{i,\ell}(t - s_{i,i} n_{i,i}) - x a_{i,\ell} + \sum_{j=p+1}^{q} \frac{x^2 \langle \alpha_{j,i}, \alpha_{j,\ell} \rangle}{t - x\lambda_j}, \tag{29}$$

and

$$\mathfrak{B}_{i,\ell} = \delta_{i,\ell}(t - s_{i,i} n_{i,i}) - x b_{i,\ell} + \sum_{j=p+1}^{q} \frac{x^2 \langle \beta_{j,i}, \beta_{j,\ell} \rangle}{t - x\lambda_j}, \tag{30}$$

where $\delta_{i,\ell}$ is the Kronecker delta function, namely

$$\delta_{i,\ell} = \begin{cases} 1, & i = \ell, \\ 0, & i \neq \ell. \end{cases} \tag{31}$$

Expand Eq. (26) with $K = \{2, 3, \ldots, p\}$, and we get

$$\det(tI - x\hat{A}_1)_{[\{2,3,\ldots,p\}],[\{2,3,\ldots,p\}]} = \mathfrak{A}_{1,1} \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j} \tag{32}$$

and

$$\det(tI - s_1\hat{B}_1)_{[\{2,3,\ldots,p\}],[\{2,3,\ldots,p\}]} = \mathfrak{B}_{1,1} \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j}. \tag{33}$$

We conclude that $a_{1,1} = b_{1,1}$ and $\langle \alpha_{j,1}, \alpha_{j,1} \rangle = \langle \beta_{j,1}, \beta_{j,1} \rangle$ for $j = p, p+1, \ldots, q$. Similarly, we have $a_{i,i} = b_{i,i}$ and $\langle \alpha_{j,i}, \alpha_{j,i} \rangle = \langle \beta_{j,i}, \beta_{j,i} \rangle$ for $i = 1, 2, \ldots, p$ and $j = p, p+1, \ldots, q$. Now we expand Eq. (26) with $K = \{3, 4, \ldots, p\}$ and get

$$\det(tI - x\hat{A}_1)_{[\{3,4,\ldots,p\}],[\{3,4,\ldots,p\}]} \tag{34}$$

$$= (\mathfrak{A}_{1,1}\mathfrak{A}_{2,2} - \mathfrak{A}_{1,2}\mathfrak{A}_{2,1}) \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j}, \tag{35}$$

and

$$\det(tI - x\hat{B}_1)_{[\{3,4,\ldots,p\}],[\{3,4,\ldots,p\}]} \tag{36}$$

$$= (\mathfrak{B}_{1,1}\mathfrak{B}_{2,2} - \mathfrak{B}_{1,2}\mathfrak{B}_{2,1}) \prod_{j=p+1}^{q} (t - x\lambda_j)^{m_j}. \tag{37}$$

Therefore,

$$\mathfrak{A}_{1,1}\mathfrak{A}_{2,2} - \mathfrak{A}_{1,2}\mathfrak{A}_{2,1} = \mathfrak{B}_{1,1}\mathfrak{B}_{2,2} - \mathfrak{B}_{1,2}\mathfrak{B}_{2,1}. \tag{38}$$

Consider the polynomial term, and we get

$$(t - xa_{11} - s_{11}n_{11})(t - xa_{22} - s_{22}n_{22}) - (-xa_{12} - s_{12}n_{12})(-xa_{21} - s_{21}n_{21}) \tag{39}$$

$$=(t - xb_{11} - s_{11}n_{11})(t - xb_{22} - s_{22}n_{22}) - (-xb_{12} - s_{12}n_{12})(-xb_{21} - s_{21}n_{21}). \tag{40}$$

Hence, $a_{1,2} = b_{1,2}$ and $a_{2,1} = b_{2,1}$. Similarly, we have $a_{i,j} = b_{i,j}$ for $1 \leq i, j \leq p$. Consider the coefficient of $\frac{1}{t - x\lambda_j}$, and we get

$$(t - xa_{11} - s_{11}n_{11})(x^2\langle \alpha_{j2}, \alpha_{j2} \rangle) + (t - xa_{22} - s_{22}n_{22})(x^2\langle \alpha_{j1}, \alpha_{j1} \rangle) \tag{41}$$

$$- (-xa_{12})(x^2\langle \alpha_{j2}, \alpha_{j1} \rangle) - (-xa_{21})(x^2\langle \alpha_{j1}, \alpha_{j2} \rangle) \tag{42}$$

$$=(t - xb_{11} - s_{11}n_{11})(x^2\langle \beta_{j2}, \beta_{j2} \rangle) + (t - xb_{22} - s_{22}n_{22})(x^2\langle \beta_{j1}, \beta_{j1} \rangle) \tag{43}$$

$$- (-xb_{12})(x^2\langle \beta_{j2}, \beta_{j1} \rangle) - (-xb_{21})(x^2\langle \beta_{j1}, \beta_{j2} \rangle). \tag{44}$$

Hence, $a_{12}\langle \alpha_{j1}, \alpha_{j2}\rangle = b_{12}\langle \beta_{j1}, \beta_{j2}\rangle$ for $j = p+1, p+2, \dots, q$. Consider the coefficient of $\frac{1}{(t-x\lambda_j)^2}$, and we get

$$x^4(\alpha_{j1}^\top \alpha_{j1}\alpha_{j2}^\top \alpha_{j2} - \langle \alpha_{j1}, \alpha_{j2}\rangle^2) = x^4(\beta_{j1}^\top \beta_{j1}\beta_{j2}^\top \beta_{j2} - \langle \beta_{j1}, \beta_{j2}\rangle^2). \tag{45}$$

Hence, $\langle \alpha_{j1}, \alpha_{j2}\rangle^2 = \langle \beta_{j1}, \beta_{j2}\rangle^2$ for $j = p+1, p+2, \dots, q$. Therefore,

$$\begin{cases} a_{12} = b_{12}, \\ \langle \alpha_{j1}, \alpha_{j2}\rangle = \langle \beta_{j1}, \beta_{j2}\rangle, \quad j = p+1, p+2, \dots, q \end{cases} \tag{46}$$

or

$$\begin{cases} a_{12} = -b_{12}, \\ \langle \alpha_{j1}, \alpha_{j2}\rangle = -\langle \beta_{j1}, \beta_{j2}\rangle, \quad j = p+1, p+2, \dots, q \end{cases} \tag{47}$$

In the latter case, consider $N = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & I \end{bmatrix}$ and $N^\top \hat{B}_1 N$, then it reduces to the first case. Similarly, we get $a_{i,j} = \pm b_{i,j}$, $i, j = 1, 2, \dots, p$ and

$$\langle \alpha_{j,i}, \alpha_{j,\ell}\rangle = \pm\langle \beta_{j,k}, \beta_{j,\ell}\rangle, \quad j = p+1, p+2, \dots, q, \quad i, \ell = 1, 2, \dots, p. \tag{48}$$

Next we try to show that the minus sign case can be reduced to positive sign case consistently. We can turn the minus sign case to the positive sign case sequentially and get $a_{12} = b_{12}, a_{23} = b_{23}, \dots, a_{p-1,p} = b_{p-1,p}$. Consequently, $\langle \alpha_{j,i}, \alpha_{j,i+1}\rangle = \langle \beta_{j,i}, \beta_{j,i+1}\rangle$ for $i = 1, 2, \dots, p-1$ and $j = p+1, p+2, \dots, q$. We expand Eq. (26) with $K = L = \{4, 5, \dots, p\}$ and get

$$\begin{aligned}
&\mathfrak{A}_{1,1}\mathfrak{A}_{2,2}\mathfrak{A}_{3,3} + \mathfrak{A}_{1,2}\mathfrak{A}_{2,3}\mathfrak{A}_{3,1} + \mathfrak{A}_{1,3}\mathfrak{A}_{2,1}\mathfrak{A}_{3,2} && (49)\\
&\quad - \mathfrak{A}_{1,3}\mathfrak{A}_{2,2}\mathfrak{A}_{3,1} - \mathfrak{A}_{1,2}\mathfrak{A}_{2,1}\mathfrak{A}_{3,3} - \mathfrak{A}_{1,1}\mathfrak{A}_{2,3}\mathfrak{A}_{3,2} && (50)\\
=&\mathfrak{B}_{1,1}\mathfrak{B}_{2,2}\mathfrak{B}_{3,3} + \mathfrak{B}_{1,2}\mathfrak{B}_{2,3}\mathfrak{B}_{3,1} + \mathfrak{B}_{1,3}\mathfrak{B}_{2,1}\mathfrak{B}_{3,2} && (51)\\
&\quad - \mathfrak{B}_{1,3}\mathfrak{B}_{2,2}\mathfrak{B}_{3,1} - \mathfrak{B}_{1,2}\mathfrak{B}_{2,1}\mathfrak{B}_{3,3} - \mathfrak{B}_{1,1}\mathfrak{B}_{2,3}\mathfrak{B}_{3,2}. && (52)
\end{aligned}$$

Consider the terms without t, and we obtained

$$\begin{aligned}
&(a_{11} - s_{11}n_{11})(a_{22} - s_{22}n_{22})(a_{33} - s_{33}n_{33}) + (a_{12})a_{23}a_{31} + a_{13}a_{21}a_{32} && (53)\\
&\quad - a_{1,3}(a_{2,2} - s_3n_3)a_{3,1} - a_{1,2}a_{2,1}(a_{3,3} - s_4n_4) - (a_{1,1} - s_2n_2)a_{2,3}a_{3,2} && (54)\\
&(b_{1,1} - s_2n_2)(b_{2,2} - s_3n_3)(b_{3,3} - s_4n_4) + b_{1,2}b_{2,3}b_{3,1} + b_{1,3}b_{2,1}b_{3,2} && (55)\\
&\quad - b_{1,3}(b_{2,2} - s_3n_3)b_{3,1} - b_{1,2}b_{2,1}(b_{3,3} - s_4n_4) - (b_{1,1} - s_2n_2)b_{2,3}b_{3,2}. && (56)
\end{aligned}$$

Note that we have $a_{i,i} = b_{i,i}$ for $i = 1, 2, 3$, and $a_{1,2} = b_{1,2} = a_{2,1} = b_{2,1}, a_{2,3} = b_{2,3} = a_{3,2} = b_{3,2}$, so

$$(a_{1,3} - b_{1,3})((a_{1,3} + b_{1,3})(a_{2,2} - s_3n_3) - 2a_{1,2}a_{3,2}) = 0. \tag{57}$$

Therefore,

$$a_{1,3} = b_{1,3}, \tag{58}$$

or

$$\begin{cases} a_{1,3} = -b_{1,3}, \\ a_{1,2}a_{3,2} = 0. \end{cases} \tag{59}$$

Note that by assumption $a_{1,2} = \frac{e_1^\top}{\|e_1\|} A_1 \frac{e_2}{\|e_2\|} \neq 0$ and $a_{3,2} = \frac{e_3^\top}{\|e_3\|} A_1 \frac{e_2}{\|e_2\|} \neq 0$. So $a_{1,3} = b_{1,3} = \frac{e_1^\top}{\|e_1\|} A_1 \frac{e_3}{\|e_3\|} \neq 0$. Similarly, we have $a_{i,j} = b_{i,j} =$ for $1 < |i-j| \leq p-1$. Altogether, we have

$$\langle \alpha_{j,i}, \alpha_{j,\ell} \rangle = \langle \beta_{j,k}, \beta_{j,\ell} \rangle, \quad j = p+1, p+2, \ldots, q, \quad i, \ell = 1, 2, \ldots, p. \tag{60}$$

Therefore, there exists an orthogonal matrix $R = \begin{bmatrix} I_p & 0 \\ 0 & V \end{bmatrix}$ such that $\hat{A}_1 = R^\top \hat{B}_1 R$. Consider $Q = OR$ (or $Q = ONR$ if $p = 2$), then $Q^\top W_{\boldsymbol{A}}(\boldsymbol{s}) Q = W_{\boldsymbol{B}}(\boldsymbol{s})$, and it satisfies the conditions in the theorem. □

Definition 2.4. *Let $G = (V, E)$ be a graph. A graph-vector of G is a vector $\xi_G \in \mathbb{R}^V$ such that it is invariant under the automorphisms of G, namely if P is a permutation matrix such that $P^\top A_G P = A_G$, then $\xi_G = P^\top \xi_G$.*

Lemma 2.5. *Let $G = (V, E)$ be a graph. Then all the graph-vectors of G form a linear subspace of $\mathbb{R}^V$, whose dimension is equal to the number of orbits of* $\mathrm{Aut}(G)$. *More precisely, the graph-vectors of G are those which take constant value within an orbit.*

Proof. We construct a basis of graph-vectors directly. Let (G, x_0) be a rooted graph where $x_0 \in V$. Consider the vector $\xi_{G,x_0} \in \mathbb{R}^V$ as follows.

$$\xi_{G,x_0}(x) = \begin{cases} 1, & (G, x) \cong (G, x_0) \\ 0, & (G, x) \ncong (G, x_0). \end{cases} \tag{61}$$

It is clear that ξ_{G,x_0} is invariant under the action of $\mathrm{Aut}(G)$. Therefore, ξ_{G,x_0} is indeed a graph-vector. Moreover, $\xi_{G,x_0} = \xi_{G,x_0'}$ if x_0 and x_0' are in the same orbit of $\mathrm{Aut}(G)$.

Note that a graph-vector is invariant under the action of $\mathrm{Aut}(G)$, therefore it is a linear combination of ξ_{G,x_0} with $x_0 \in V$. We conclude that $\{\xi_{G,x_0}, x_0 \in V\}$ gives a basis of graph-vectors, whose size is equal to the number of orbits of $\mathrm{Aut}(G)$. □

Lemma 2.6. *Let Q be a rational matrix and U be a unimodular matrix. Then $\ell(Q) = \ell(QU)$.*

Proof. Suppose $R = QU$. Then $\ell(Q)R = \ell(Q)QU$ is an integral matrix. Therefore, $\ell(R) \mid \ell(Q)$. On the other hand, $Q = RU^{-1}$ and U^{-1} is unimodular. Therefore, $\ell(Q) \mid \ell(R)$. Altogether, we get $\ell(Q) = \ell(QU)$. □

Lemma 2.7. *Let X and Y be two $n \times m$ integral matrices ($n \leq m$) and let Q be a square matrix of order n. Suppose $QX = Y$ and X is of full row rank. Then Q is a unique rational matrix and $\ell(Q) \mid d_n(X)$, where $d_n(X)$ is the last invariant factor of X.*

Proof. For each row $q^\top$ of Q and the corresponding row $y^\top$ of Y, we have $q^\top X = y^\top$. Since X is of full rank and both X and Y are integral matrices, the row $q^\top$ is determined by X and Y, and it is rational. Hence, Q is a unique rational matrix. Consider the Smith decomposition of X, namely $X = U\Sigma V$, where both U and V are unimodular matrices. Then $QU\Sigma V = Y$. Hence, $QU\Sigma = YV^{-1}$ is integral. Note that $d_n(X) = d_n(\Sigma)$. Hence, $\ell(Q) = \ell(QU) \mid d_n(\Sigma) = d_n(X)$. □

Lemma 2.8 ([WY16, Lemma 4.5])**.** *Let Q be a rational orthogonal matrix, A a symmetric integral matrix, such that $Q^\top AQ$ is a symmetric integral matrix. Suppose p is an odd prime, $p \mid \ell(Q)$, and $p \mid \Delta_A$, where Δ_A is the discriminant of A. Then $p^2 \mid \Delta_A$.*

3 The Weisfeiler-Lehman algorithm

Let $A : V \times V \to C$ be a square matrix indexed by V, whose entries take value in a set C. We define an equivalence relation on the set of k-tuples in V^k. Let $\mathcal{U}_k$ be the set of all such k-tuples. Two k-tuples $(i_1, i_2, \ldots, i_k)$ and $(j_1, j_2, \ldots, j_k)$ are equivalent if

1. $i_\ell = i_{\ell'}$ if and only if $j_\ell = j'_\ell$,
2. $A(i_\ell, i_{\ell'}) = c$ if and only if $A(j_\ell, j_{\ell'}) = c$.

We define the atomic type $\operatorname{atp}(i_1, i_2, \ldots, i_k) = \operatorname{atp}_A(i_1, i_2, \ldots, i_k)$ of a k-tuple as its equivalence class. The information of atomic type $\operatorname{atp}(i_1, i_2, \ldots, i_k)$ can be encoded in a $k \times k$ matrix T with

$$T_{p,q} = T(A,k)_{p,q} = \begin{cases} (0, A(i_p, i_q)), & i_p = i_q, \\ (1, A(i_p, i_q)), & i_p \neq i_q. \end{cases} \tag{62}$$

Let S_1 be the set of all different types of k-tuples, and it is the set of initial colors. We define the set S of colors by

$$S = \bigcup_{k=1}^{\infty} S_k, \tag{63}$$

where elements of S_{r+1} are finite multisets, which can be regarded as formal sums, of finite sequences whose elements are in $\cup_{k=1}^{r} S_k$. In fact, it is enough to work with as many colors as k-tuples by renaming the colors in each round.

The k-WL algorithm works by iteratively assign colors to $\mathcal{U}_k$. That is to say, we define the functions $X^r_{A,k} : \mathcal{U}_k \to S$. For $r = 1$, we define

$$X^1_{A,k}(i_1 \ldots i_k) = \operatorname{atp}_A(i_1 \ldots i_k). \tag{64}$$

Sequentially we have

$$X^{r+1}_{A,k}(i_1 \dots i_k) = \left(X^r_{A,k}(i_1 \dots i_k), \sum_{m \in V} (\mathrm{atp}_A(i_1 \dots i_k m), S^r_{A,k}(i_1 \dots i_k m)) \right), \tag{65}$$

where $S^r_{A,k}(i_1 \dots i_k m)$ is the sequence

$$(X^r_{A,k}(i_1 \dots i_{k-1} m), \dots, X^r_{A,k}(i_1 \dots i_{\ell-1} m i_{\ell+1} \dots i_k), \dots, X^r_{A,k}(m i_2 \dots i_k)) \tag{66}$$

The summation in Eq. (65) is regarded as a formal sum.

Note that $X^r_{A,k}$ induces a partition $\mathcal{P}(A,k,r)$ of the set $\mathcal{U}_k$ of k-tuples for each $r \geq 1$. In particular, atp_A, in other words $X^1_{A,k}$, induces a partition, denoted by $\mathcal{P}(A,k)$. The partition sequence stabilizes for sufficiently large r, denoted by $\mathcal{P}(A,k,\infty)$. We define the closure $\mathrm{cl}(P)$ of $P = \mathcal{P}(A,k)$ as $\mathcal{P}(A,k,\infty)$. There is a partial order among the partitions of $\mathcal{U}_k$. Let P_1, P_2 be two partitions of a set X. We say P_1 is finer than P_2, or P_2 is coarser than P_1, denoted by $P_1 \trianglelefteq P_2$, if every part of P_1 is contained in a part of P_2. Note that

$$\mathcal{P}(A,k) = \mathcal{P}(A,k,1) \trianglerighteq \mathcal{P}(A,k,2) \trianglerighteq \cdots \trianglerighteq \mathcal{P}(A,k,r) \trianglerighteq \cdots \trianglerighteq \mathcal{P}(A,k,\infty) = \mathrm{cl}(\mathcal{P}(A,k)). \tag{67}$$

We write $x \overset{P}{\sim} y$ if x and y are in the same part of P.

We define an invariant to record the result of k-WL coloring.

$$I_{A,k}(t) \coloneqq \sum_{r=0}^{\infty} t^r M^r_{A,k}, \tag{68}$$

where

$$M^r_{A,k} = \sum_{(i_1 \dots i_k) \in \mathcal{U}_k} X^r_{A,k}(i_1 \dots i_k). \tag{69}$$

Proposition 3.1 (Analogue of [AIP10, Proposition 4])**.** *Let $A, B : V \times V \to C$ be two square matrices. Then $I_{A,k}(t) = I_{B,k}(t)$ if and only if there exists a permutation σ of k-tuples in $\mathcal{U}_k$ such that $X^r_{A,k}(i_1 \dots i_k) = X^r_{B,k}(\sigma(i_1 \dots i_k))$ for all $r \geq 1$. In particular,*

$$\mathrm{atp}_A(i_1 \dots i_k) = \mathrm{atp}_B(\sigma(i_1 \dots i_k)). \tag{70}$$

Proof. The '*if*' part is obvious. Conversely, assume $I_{A,k}(t) = I_{B,k}(t)$. The coefficient of t^r for $r = |V|^k$ implies the existence of a permutation σ on the set $\mathcal{U}_k$ of k-tuples such that

$$X^{|V|^k}_{A,k}(i_1 \dots i_k) = X^{|V|^k}_{B,k}(\sigma(i_1 \dots i_k)) \tag{71}$$

Then

$$X^r_{A,k}(i_1 \dots i_k) = X^r_{B,k}(\sigma(i_1 \dots i_k)) \tag{72}$$

holds for all $1 \leq r \leq |V|^k$. Since the WL refinement stabilizes after at most $|V|^k$ iterations, Eq. (72) holds for $r \geq |V|^k$. ☐

Theorem 3.2. *Let $A : V \times V \to C$ be a square matrix and let P be the partition of V^2 induced by atp_A. Suppose P' is a partition of V^2 induced by $A' : V \times V \to C'$ such that $P \trianglerighteq P' \trianglerighteq \mathrm{cl}(P)$. Then $\mathrm{cl}(P') = \mathrm{cl}(P)$. In particular, we have $X^r_{A,2}(i_1, i_2) = X^r_{A,2}(j_1, j_2)$ for all $r \geq 1$ if and only if $X^r_{A',2}(i_1, i_2) = X^r_{A',2}(j_1, j_2)$ for all $r \geq 1$.*

Proof. It is clear that $\mathrm{cl}(P) \trianglerighteq \mathrm{cl}(P')$. We only need to show that $\mathrm{cl}(P') \trianglerighteq \mathrm{cl}(P)$. Suppose $(i_1, i_2) \overset{\mathrm{cl}(P)}{\sim} (j_1, j_2)$. Then $X^r_{A,2}(i_1, i_2) = X^r_{A,2}(j_1, j_2)$ for all $r \geq 1$. By Proposition 3.1, there exists a permutation of V^2 such that

$$X^{r+1}_{A,2}(i_1, i_2) = X^{r+1}_{A,2}(\sigma(i_1, i_2)) \tag{73}$$

for all $r \geq 1$, where $(j_1, j_2) = \sigma(i_1, i_2)$. We have

$$X^r_{A,2}(i_1, i_2) = X^r_{A,2}(j_1, j_2), \tag{74}$$

and

$$\sum_{m \in V} (\mathrm{atp}(i_1, i_2, m), X^r_{A,2}(i_1, m), X^r_{A,2}(m, i_2)) = \sum_{m \in V} (\mathrm{atp}(j_1, j_2, m), X^r_{B,2}(j_1, m), X^r_{B,2}(m, j_2)). \tag{75}$$

Therefore, there exists a permutation $\tau = \tau(\sigma, i_1, i_2)$ such that

$$\mathrm{atp}_A(i_1, i_2, i_3) = \mathrm{atp}_A(j_1, j_2, \tau(i_3)), \tag{76}$$

$$X^r_{A,2}(i_1, i_3) = X^r_{A,2}(j_1, \tau(i_3)), \tag{77}$$

$$X^r_{A,2}(i_3, i_2) = X^r_{A,2}(\tau(i_3), j_2), \tag{78}$$

for all $i_3 \in V$. Since $\mathrm{atp}_A(i_1, i_2, i_3) = \mathrm{atp}_A(j_1, j_2, \tau(i_3))$, we know that the first entry (0 or 1) in $T(A', 3)_{p,q}$ is identical for (i_1, i_2, i_3) and $(j_1, j_2, \tau(i_3))$. Now we consider the second entry. Note that we have $X^r_{A,2}(i_1, i_2) = X^r_{A,2}(j_1, j_2)$, $X^r_{A,2}(i_1, i_3) = X^r_{A,2}(j_1, \tau(i_3))$, and $X^r_{A,2}(i_3, i_2) = X^r_{A,2}(\tau(i_3), j_2)$ for all $r \geq 1$. Take r sufficiently large, and we obtain $(i_1, i_2) \overset{\mathrm{cl}(P)}{\sim} (j_1, j_2)$, $(i_1, i_3) \overset{\mathrm{cl}(P)}{\sim} (j_1, \tau(i_3))$, and $(i_3, i_2) \overset{\mathrm{cl}(P)}{\sim} (\tau(i_3), j_2)$. Hence, $(i_1, i_2) \overset{P'}{\sim} (j_1, j_2)$, $(i_1, i_3) \overset{P'}{\sim} (j_1, \tau(i_3))$, and $(i_3, i_2) \overset{P'}{\sim} (\tau(i_3), j_2)$. Moreover, take $i_2 = i_1$ in Eqs. (77) and (78), and we conclude that $X^r_{A,2}(i_1, i_3) = X^r_{A,2}(j_1, j_3)$ if and only if $X^r_{A,2}(i_3, i_1) = X^r_{A,2}(j_3, j_1)$. Therefore, $\mathrm{atp}_{A'}(i_1, i_2, i_3) = \mathrm{atp}_{A'}(j_1, j_2, \tau(i_3))$. So $X^1_{A',2}(i_1, i_2) = X^1_{A',2}(j_1, j_2) = X^1_{A',2}(\sigma(i_1, i_2))$. Next, we prove that $X^r_{A',2}(i_1, i_2) = X^r_{A',2}(\sigma(i_1, i_2))$. This is indeed the case since

$$\mathrm{atp}_{A'}(i_1, i_2, i_3) = \mathrm{atp}_{A'}(j_1, j_2, \tau(i_3)), \tag{79}$$

$$X^r_{A',2}(i_1, i_3) = X^r_{A',2}(j_1, \tau(i_3)), \tag{80}$$

$$X^r_{A',2}(i_3, i_2) = X^r_{A',2}(\tau(i_3), j_2), \tag{81}$$

holds by induction. In other words, $(i_1, i_2) \overset{\mathrm{cl}(P')}{\sim} \sigma(j_1, j_2)$. We conclude that $\mathrm{cl}(P) = \mathrm{cl}(P')$. □

Theorem 3.3 (Analogue of [AIP10, Theorem 3]). *Let $A, B : V \times V \to C$ be two square matrices, where C is a (not necessarily commutative) ring. If $X^r_{A,2}(i,j) = X^r_{B,2}(p,q)$, then $(A^r)(i,j) = (B^r)(p,q)$.*

Proof. We prove by induction on the number of iteration. The case $r = 1$ is trivial. Suppose the claim is true for r. Then for $r+1$ we have

$$X^{r+1}_{A,2}(i,j) = X^{r+1}_{B,2}(p,q) \tag{82}$$

By Eq. (65), we have

$$\sum_{m\in V}(\mathrm{atp}(i,j,m), X^r_{A,2}(i,m), X^r_{A,2}(m,j)) = \sum_{m\in V}(\mathrm{atp}(p,q,m), X^r_{B,2}(p,m), X^r_{B,2}(m,q)) \tag{83}$$

Therefore there exists a permutation τ on V such that

$$\mathrm{atp}_A(i,j,m) = \mathrm{atp}_B(p,q,\tau(m)) \tag{84}$$

$$X^r_{A,2}(i,m) = X^r_{B,2}(p,\tau(m)) \tag{85}$$

$$X^r_{B,2}(m,j) = X^r_{B,2}(\tau(m),q) \tag{86}$$

By the induction hypothesis, we have

$$A(i,m) = B(p,\tau(m)) \tag{87}$$

$$A(m,j) = B(\tau(m),q) \tag{88}$$

$$(A^r)(i,m) = (B^r)(p,\tau(m)) \tag{89}$$

$$(A^r)(m,j) = (B^r)(\tau(m),q) \tag{90}$$

By summing over m, we get

$$\sum_m A(i,m)(A^r)(m,j) = \sum_m B(p,m)(B^r)(m,q) \tag{91}$$

In other words, $(A^{r+1})(i,j) = (B^{r+1})(p,q)$. □

Theorem 3.4 (Analogue of [AIP10, Theorem 4]). *Let A_1 and B_1 be two real symmetric matrices of order n. Let e_i, $i = 1,2,\dots,p$ be zero-one vectors of length n such that the positions of the ones are disjoint. Let $J_{i,j} = e_i e_j^\top$ for $i,j = 1,2,\dots,p$ and $k = 1+p^2$. Let $\boldsymbol{A} = (A_1, A_2, \dots, A_k) = (A_1, J_{1,1}, J_{1,2}, \dots, J_{p,p})$ and $\boldsymbol{B} = (B_1, B_2, \dots, B_k) = (B_1, J_{1,1}, J_{1,2}, \dots, J_{p,p})$. If $I_{W(\boldsymbol{A},\boldsymbol{s}),2}(t) = I_{W(\boldsymbol{B},\boldsymbol{s}),2}(t)$, then $\phi_{\boldsymbol{A}}(\boldsymbol{s};t) = \phi_{\boldsymbol{B}}(\boldsymbol{s};t)$.*

Proof. Assume $I_{W(\boldsymbol{A},\boldsymbol{s}),2}(t) = I_{W(\boldsymbol{B},\boldsymbol{s}),2}(t)$. By Proposition 3.1, there exists a permutation σ of the set $\mathcal{U}_2$ of 2-tuples such that for every 2-tuple (i,j), it holds

$$X^r_{W(\boldsymbol{A},\boldsymbol{s}),2}(i,j) = X^r_{W(\boldsymbol{B},\boldsymbol{s}),2}(\sigma(i,j)) \tag{92}$$

for all $r \geq 1$. For $r = 1$, we have

$$\mathrm{atp}_{W(\boldsymbol{A},\boldsymbol{s})}(i,j) = \mathrm{atp}_{W(\boldsymbol{B},\boldsymbol{s})}(\sigma(i,j)). \tag{93}$$

If $i = j$, then σ send the diagonal of $X^r_{W(\boldsymbol{A},\boldsymbol{s}),2}$ to the diagonal of $X_{W(\boldsymbol{B},\boldsymbol{s}),2}$, namely

$$\sigma(i,i) = (p,p) \tag{94}$$

for some $p \in V$. Therefore,

$$\sum_i X^r_{W(\boldsymbol{A},\boldsymbol{s}),2}(i,i) = \sum_i X^r_{W(\boldsymbol{B},\boldsymbol{s}),2}(\sigma(i,i)). \tag{95}$$

By Theorem 3.3, we get

$$\sum_i (W(\boldsymbol{A},\boldsymbol{s}))^r(i,i) = \sum_i (W(\boldsymbol{B},\boldsymbol{s}))^r(\sigma(i,i)). \tag{96}$$

In other words $\mathrm{Tr}(W(\boldsymbol{A},\boldsymbol{s})^r) = \mathrm{Tr}((W(\boldsymbol{B},\boldsymbol{s}))^r)$ for all $r \geq 1$. Then $\phi_{\boldsymbol{A}}(\boldsymbol{s};t) = \phi_{\boldsymbol{B}}(\boldsymbol{s};t)$. $\square$

Theorem 3.5. *Let G and H be two graphs on V sharing the same degree sequences. Without loss of generality, suppose $\deg(v) = \deg_G(v) = \deg_H(v)$ for all $v \in V$. Therefore, we have the degree decomposition of vertices $V = \bigsqcup_{i=1}^p V_i$. Let A and B be the adjacency matrices of G and H respectively. Let $e_i \in \mathbb{R}^V$, $i = 1, 2, \ldots, p$ be zero-one vectors such that $e_i(v) = 1$ if and only if $v \in V_i$. Let $J_{i,j} = e_i e_j^\top$ for $i, j = 1, 2, \ldots, p$. Let $D_i(u,v) = \begin{cases} 1, & u = v \in V_i, \\ 0, & \text{otherwise.} \end{cases}$ Define $A' = s_0A + s_1D_1 + \cdots + s_pD_p$ and $B' = s_0B + s_1D_1 + \cdots + s_pD_p$. Define $A'' = s_0A_0 + s_1J_{1,1} + \cdots + s_pJ_{p,p}$ and $B'' = s_0B + s_1J_{1,1} + \cdots + s_pJ_{p,p}$. Define $A''' = s_0A_0 + s_{1,1}J_{1,1} + s_{1,2}J_{1,2} + \cdots + s_pJ_{p,p}$ and $B''' = s_0B + s_{1,1}J_{1,1} + s_{1,2}J_{1,2} + \cdots + s_pJ_{p,p}$. Then the followings are equivalent.*

1. $I_{A,2}(t) = I_{B,2}(t)$.
2. $I_{A',2}(t) = I_{B',2}(t)$.
3. $I_{A'',2}(t) = I_{B'',2}(t)$.
4. $I_{A''',2}(t) = I_{B''',2}(t)$.

Proof. Let P, P', P'', P''' be the partition induced by A, A', A'', A''' respectively. By Theorem 3.2, we only need to show that $P \trianglerighteq P' \trianglerighteq \mathrm{cl}(P)$ and $P \trianglerighteq P'' \trianglerighteq P''' \trianglerighteq \mathrm{cl}(P)$ since the case for B is identical. Suppose $(u,v) \overset{\mathrm{cl}(P)}{\sim} (z,w)$. By Proposition 3.1, there exists a permutation σ of 2-tuples such that

$$X^r_{A,2}(u,v) = X^r_{A,2}(z,w) \tag{97}$$

for all $r \geq 1$, where $(z, w) = \sigma(u, v)$ for $(u, v) \in V^2$. By Theorem 3.3, we have $(A^r)(u, v) = (A^r)(z, w)$. Note that σ maps the diagonal of $X^r_{A,2}$ to diagonal of $X^r_{A,2}$. In particular, we have $\deg(u) = (A^2)(u, u) = (A^2)(z, z) = \deg(z)$. Therefore, we have $\sigma(\mathrm{diag}(V_i^2)) = \mathrm{diag}(V_i^2)$ for $i = 1, 2, \ldots, p$, where $\mathrm{diag}(V_i^2) \coloneqq \{(v, v) \in V_i^2\}$. We conclude that $P \trianglerighteq P' \trianglerighteq \mathrm{cl}(P)$.

It is clear that $\sigma(\mathrm{offdiag}(V^2)) = \mathrm{offdiag}(V^2)$, where $\mathrm{offdiag}(V^2) \coloneqq \{(u, v) \in V^2 \mid u \neq v\}$. We claim that $\sigma(\mathrm{offdiag}(V_i^2)) = \mathrm{offdiag}(V_i^2)$ for $i = 1, 2, \ldots, p$, where $\mathrm{offdiag}(V_i^2) \coloneqq \{(u, v) \in V_i^2 \mid u \neq v\}$. Suppose $(u_1, u_2) \in \mathrm{offdiag}(V_i^2)$ and $\sigma(u_1, u_2) = (z_1, z_2)$. Take $r = 3$, and expand

$$X^3_{A,2}(u, v) = X^3_{A,2}(z, w). \tag{98}$$

We get

$$\begin{aligned} &\sum_{m \in V} (\mathrm{atp}_A(u_1, u_2, m), X^2_{A,2}(u_1, m), X^2_{A,2}(m, u_2)) && (99) \\ = &\sum_{m \in V} (\mathrm{atp}_A(z_1, z_2, m), X^2_{A,2}(z_1, m), X^2_{A,2}(m, z_2)). && (100) \end{aligned}$$

Therefore, there exists a permutation τ of V such that

$$\begin{aligned} &(\mathrm{atp}_A(u_1, u_2, m), X^2_{A,2}(u_1, m), X^2_{A,2}(m, u_2)) && (101) \\ = &(\mathrm{atp}_A(z_1, z_2, \tau(m)), X^2_{A,2}(z_1, \tau(m)), X^2_{A,2}(\tau(m), z_2)). && (102) \end{aligned}$$

We claim $\tau(u_1) = z_1$ and $\tau(u_2) = z_2$. In fact, $X^2_{A,2}(u_1, u_1) = X^2_{A,2}(z_1, \tau(u_1))$ implies $\mathrm{atp}_A(u_1, u_1) = \mathrm{atp}_A(z_1, \tau(u_1))$. Hence, $\tau(u_1) = z_1$. Similarly, $\tau(u_2) = z_2$. In particular, we get $X^2_{A,2}(u_1, u_1) = X^2_{A,2}(z_1, z_1)$, thus $\deg(u_1) = A^2(u_1, u_1) = A^2(z_1, z_1) = \deg(z_1)$. Therefore, $z_1 \in V_i$. Similarly, $z_2 \in V_i$. We conclude that $\sigma(\mathrm{offdiag}(V_i^2)) = \mathrm{offdiag}(V_i^2)$, thus $\sigma(V_i^2) = V_i^2$.

Next we claim that $\sigma(V_i \times V_j) = V_i \times V_j$ for $1 \leq i \neq j \leq p$. Suppose $(u_1, u_2) \in V_i \times V_j$ and $\sigma(u_1, u_2) = (z_1, z_2)$. By similar argument we get $z_1 \in V_i$ and $z_2 \in V_j$. Therefore, $\sigma(V_i \times V_j) = V_i \times V_j$ for $1 \leq i \neq j \leq p$. Hence, we obtain $P \trianglerighteq P'' \trianglerighteq P''' \trianglerighteq \mathrm{cl}(P)$. □

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References

[AIP10] Afredo Alzaga, Rodrigo Iglesias, and Ricardo Pignol. Spectra of symmetric powers of graphs and the Weisfeiler–Lehman refinements. *Journal of Combinatorial Theory, Series B*, 100(6):671–682, November 2010.

[WY16] Wei Wang and Tao Yu. Square-free Discriminants of Matrices and the Generalized Spectral Characterizations of Graphs. *arXiv:1608.01144 [math]*, August 2016. arXiv: 1608.01144 version: 1.