High-order spectral characterizations of graphs

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Abstract

The tensor spectra of the power hypergraph of a graph G is called the high-order spectra of G. In this paper, we show that all Smith graphs are determined by their high-order spectra. We give some high-order cospectral invariants of trees and use them to show that some cospectral trees constructed by the classical Schwenk method can be distinguished by their high-order spectra.

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1. Introduction

If there was a "Holy Grail" in graph theory, it would be a practical test for graph isomorphism [18]. It was commonly believed that two cospectral graphs are isomorphic [13], until a pair of non-isomorphic cospectral trees was presented by Collatz and Sinogowitz in 1957 [24]. Many non-isomorphic cospectral graphs have since been found [8, 12, 20].

If all graphs who are cospectral with a graph G are isomorphic to G, the graph G is said to be *determined by the spectra* (short for *DS*). Until now, the known DS graphs are very special [9, 22, 23, 25].

There have been several variants of research on spectral characterization of graphs and researchers used many kinds of spectra to study them, such as the Laplacian spectra [17, 18], the generalized spectra [25] and the Hermitian spectra [26, 27].

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Let the k-power hypergraph $G^{(k)}$ be the k-uniform hypergraph that is obtained by adding $k-2$ new vertices to each edge of G for $k \geq 2$ [14]. The spectra of $G^{(k)}$ is called the *k-order spectra* of G. Some interesting properties of the k-order spectra of G are given, for example, the k-order spectra of G is always k-symmetric [10] and the k-order eigenvalues of G can be generated from the eigenvalues of signed subgraphs of G for $k \geq 3$ [4]. If graphs G_1 and G_2 have the same k-order spectra for some k, G_1 and G_2 are said to be *k-order cospectral.* If graphs which have the same k-order spectra with the graph G are isomorphic to G, we say that G is *determined by the k-order spectra.* If G_1 and G_2 are k-order cospectral for all positive integers $k \geq 2$, G_1 and G_2 are said to be *high-order cospectral.*

Definition 1.1. *A graph G is* determined by the high-order spectra *(DHS for short) if all graphs who are high-order cospectral with G are isomorphic to G.*

Notice that the graphs determined by the k-order spectra for some k are DHS and then the graphs determined by the spectra (2-order spectra) are DHS.

In 1970, Smith classified all connected graphs with spectral radii at most 2 [21], which usually are called "Smith graphs". In 2009, Van Dam and Haemers gave all graphs which are not determined by the spectra in the Smith's classification [23]. We show that these graphs given by Van Dam and Haemers are determined by the high-order spectra, thus all Smith graphs are determined by the high-order spectra. In 1973, Schwenk gave a useful method to construct non-isomorphic cospectral trees and proved his famous conclusion: "Almost all trees are not DS" [20]. We show that the infinitely many pairs of non-isomorphic cospectral trees constructed by Schwenk's method have different high-order spectra. That means these trees cannot be distinguished by the spectra, but our results show that they can be distinguished by the high-order spectra.

This paper is organized as follows. In Section 2, we introduce the spectra of hypergraphs and some lemmas. In Section 3, we show that Smith graphs are determined by the high-order spectra. In Section 4, we give some high-order cospectral invariants about the number of some subtrees. Using these high-order cospectral invariants, we give infinitely many pairs of cospectral trees with different high-order spectra.

2. Preliminaries

In this section, we introduce the spectra of a hypergraph and present lemmas which are important to the results of this paper. For a positive integer n, let $[n] =$

$\{1,\ldots,n\}$. A k-order n-dimension complex tensor $T=(t_{i_1\cdots i_k})$ is a multidimensional array with n^k entries on complex number field $\mathbb{C}$, where $i_j\in[n]$, $j=1,\ldots,k$. Denote the set of n-dimension complex vectors by $\mathbb{C}^n$. For $x=(x_1,\ldots,x_n)^{\mathrm{T}}\in\mathbb{C}^n$, Tx^{k-1} denotes a vector in $\mathbb{C}^n$ whose i-th component is

$$\left(Tx^{k-1}\right)_i=\sum_{i_2,\ldots,i_k=1}^{n} t_{ii_2\cdots i_k}x_{i_2}\cdots x_{i_k}.$$

If there exist $\lambda\in\mathbb{C}$ and a nonzero vector $x=(x_1,x_2,\ldots,x_n)^{\mathrm{T}}\in\mathbb{C}^n$ such that $Tx^{k-1}=\lambda x^{[k-1]}$, then λ is called an *eigenvalue* of T and x is an *eigenvector* of T corresponding to λ, where $x^{[k-1]}=\left(x_1^{k-1},\ldots,x_n^{k-1}\right)^{\mathrm{T}}$ [16, 19].

A hypergraph $H=(V(H),E(H))$ is called *k-uniform* if each edge of H contains exactly k vertices. For a k-uniform hypergraph H with n vertices, its (normalized) *adjacency tensor* $A_H=(a_{i_1i_2\ldots i_k})$ is a k-order n-dimension tensor [6], where

$$a_{i_1i_2\ldots i_k}=\begin{cases}\frac{1}{(k-1)!}, & \text{if } \{i_1,i_2,\ldots,i_k\}\in E(H),\\ 0, & \text{otherwise.}\end{cases}$$

All the eigenvalues of A_H are called the *spectra* of the hypergraph H [6]. When H is 2-uniform, A_H is the adjacency matrix of the graph H.

A signed graph G^π is a pair (G,π), where $G=(V,E)$ is a graph and the edge sign function is $\pi:E\to\{+1,-1\}$. We use $i\sim j$ to denote that the vertices i and j are adjacent in the graph G and use $\pi(i,j)$ to denote the sign of edge $\{i,j\}$. The adjacency matrix $A(G^\pi)=(A_{ij})$ of the signed graph G^π is the symmetric $\{0,+1,-1\}$-matrix, where

$$A_{ij}=\begin{cases}\pi(i,j), & \text{if } i\sim j,\\ 0, & \text{otherwise.}\end{cases}$$

The eigenvalues of $A(G^\pi)$ are called the eigenvalues of G^π. An (induced) subgraph of the signed graph G^π is called a signed (induced) subgraphs of G. All the eigenvalues of $G^{(k)}$ without counting multiplicity were given by the eigenvalues of signed subgraphs of G as follows [4].

Lemma 2.1. *[4] Let $G^{(k)}$ be the k-power hypergraph of a graph G.*
(1) When $k=3$, λ is an eigenvalue of $G^{(3)}$ if and only if there is a signed induced subgraph with an eigenvalue β such that $\beta^2=\lambda^k$.

(2) When $k > 3$, λ is an eigenvalue of $G^{(k)}$ if and only if there is a signed subgraph with an eigenvalue β such that $\beta^2 = \lambda^k$.

In [2], the authors gave the characteristic polynomial of power hyperpaths and provided a closed formula of their distinct eigenvalues.

Lemma 2.2. *[2] The set of all distinct eigenvalues of the k-uniform hyperpath $P_n^{(k)}$ is*

$$\left\{\lambda \in \mathbb{C} : \lambda^k = \left(2\cos\frac{\pi}{j+1}t\right)^2, j \in [n], t \in [j]\right\}.$$

A signed cycle (C_n, π) is called positive (resp. negative) cycle if the product of signs of all edges of (C_n, π) is positive (resp. negative). We use C_n^+ and C_n^- to denote the positive and negative cycle, respectively. Since the connected subgraphs of the cycle C_n are C_n and P_j for $j \in [n-1]$, we obtain all distinct eigenvalues of $C_n^{(k)}$ from all eigenvalues of C_n^+, C_n^- and P_j by Lemma 2.1. This result will be used to find distinct eigenvalues of power hypergraphs of Smith graphs and their cospectral graphs in Section 3.

Lemma 2.3. *The set of all distinct eigenvalues of the k-power hypercycle $C_n^{(k)}$ (for $k > 3$) is*

$$\left\{\lambda \in \mathbb{C} : \lambda^k = \beta^2, \beta \in \Omega\right\},$$

where

$$\Omega = \{2\cos\frac{t\pi}{j+1}, 2\cos\frac{2r\pi}{n}, 2\cos\frac{(2r-1)\pi}{n} : j \in [n-1], t \in [j], r \in [n]\}.$$

Proof. The connected subgraphs of cycle C_n are C_n and P_j for $j \in [n-1]$. By Lemmas 2.1 and 2.2, we know that the complex number λ is an eigenvalue of the k-power hypercycle $C_n^{(k)}$ (for $k > 3$) if and only if there is

$$\beta \in \{2\cos\frac{t\pi}{j+1} : j \in [n-1], t \in [j]\} \cup \sigma(C_n^+) \cup \sigma(C_n^-)$$

such that $\lambda^k = \beta^2$, where $\sigma(C_n^+)$ (resp. $\sigma(C_n^-)$) is the set of all eigenvalues of C_n^+ (resp. C_n^-). It is known that $\sigma(C_n^+) = \{2\cos\frac{2\pi r}{n} : r \in [n]\}$ [9, Page 72] and $\sigma(C_n^-) = \{2\cos\frac{(2r-1)\pi}{n} : r \in [n]\}$ [11, Lemma 2.3], then we have

$$\beta \in \{2\cos\frac{t\pi}{j+1}, 2\cos\frac{2r\pi}{n}, 2\cos\frac{(2r-1)\pi}{n} : j \in [n-1], t \in [j], r \in [n]\}.$$

□

The *d-th order spectral moment* $\mathrm{S}_d(G)$ of a graph G is the sum of d-th power of all eigenvalues of G. Two graphs are cospectral if and only if all of their d-th order spectral moments are equal [23]. The spectral moment of a graph is an important parameter in spectral characterizations of graphs [1, 7, 15, 22]. Let $\widehat{G}$ be a connected subgraph of G. We use $N_G(\widehat{G})$ to denote the number of subgraphs of G isomorphic to $\widehat{G}$.

A walk is a sequence of vertices and edges of a graph, and a walk is said to be closed if the beginning and ending vertices are identical [7]. We use $c_d(\widehat{G})$ to denote the number of closed walks with length d in the graph $\widehat{G}$ running through all the edges at least once. The d-th order spectral moment $\mathrm{S}_d(G)$ can be represented as a linear combination of the number of connected subgraphs [1, 7, 9], i.e.,

$$\mathrm{S}_d(G) = \sum\nolimits_{\widehat{G}\in G(d)} c_d(\widehat{G}) N_G(\widehat{G}),$$

where $G(d)$ is the set of connected subgraphs of G with at most d edges. The coefficient $c_d(\widehat{G})$ is called the *d-th order spectral moment coefficient of* $\widehat{G}$. A formula for the d-th order spectral moment coefficients of trees was given in [3].

Lemma 2.4. *[3, Theorem 2.10] The d-th order spectral moment of the tree T is*

$$\mathrm{S}_d\left(T\right) = \begin{cases} \sum\limits_{m=1}^{\frac{d}{2}} \sum\limits_{\widehat{T}\in \mathbf{T}(m)} c_d(\widehat{T}) N_T(\widehat{T}), & 2 \mid d, \\ 0, & 2 \nmid d, \end{cases}$$

where $\mathbf{T}(m)$ *is the set of subtrees of* T *with* m *edges. The d-th order spectral moment coefficient of the subtree* $\widehat{T}$ *is*

$$c_d(\widehat{T}) = \begin{cases} d \sum\limits_{\sum_{e\in E(\widehat{T})} w(e) = \frac{d}{2}} \left(\prod\limits_{e\in E(\widehat{T})} w(e) \prod_{v\in V(\widehat{T})} \frac{(d_v-1)!}{r_v} \right), & 2 \mid d, \\ 0, & 2 \nmid d, \end{cases} \tag{2.1}$$

where $w(e)$ *is a positive integer corresponding to edge* e *of the tree* $\widehat{T}$, $r_v = \prod_{e\in E_v(\widehat{T})} w(e)!$ *and* $d_v = \sum_{e\in E_v(\widehat{T})} w(e)$.

Similar to the spectral moments of graphs, the d-th order spectral moment $\mathrm{S}_d(H)$ of a k-uniform hypergraph H is the sum of d-th power of all eigenvalues of H, i.e., $\mathrm{S}_d(H) = \sum_{\lambda\in\sigma(H)} \lambda^d$, where $\sigma(H)$ is the spectra of H. Two hypergraphs are cospectral if and only if their d-th order spectral moments are equal for all $d \geq 1$ [5]. Clark and Cooper expressed the characteristic polynomial coefficients of a uniform hypergraph H by means of the spectral moments of H and gave the "Harary-Sachs Theorem" of hypergraphs [5]. In [3], the authors expressed the spectral moment of power hypertree by the number of subtrees as follows.

Lemma 2.5. *[3] Let $T^{(k)}$ be the k-power hypertree of a tree T. Let $c_i(\widehat{T})$ denote the i-th order spectral moment coefficient of the subtree $\widehat{T}$. Then the d-th spectral moment of $T^{(k)}$ is*

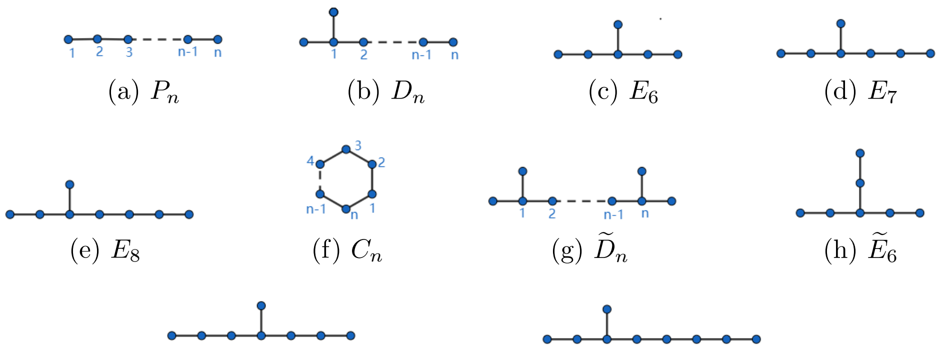
$$\mathrm{S}_d\left(T^{(k)}\right) = \begin{cases} \sum\limits_{m=1}^{\frac{d}{k}} \frac{1}{2}(k-1)^{(|E(T)|-m)(k-1)} k^{m(k-2)+1} \sum\limits_{\widehat{T}\in\mathbf{T}(m)} c_{\frac{2d}{k}}(\widehat{T}) N_T(\widehat{T}), & k \mid d, \\ 0, & k \nmid d, \end{cases}$$

where $\mathbf{T}(m)$ is the set of subtrees of T with m edges.

3. Smith graphs are DHS

Connected graphs with spectral radii at most 2 are usually called "Smith graphs", since Smith classified them in 1970 [21]. In 2009, Van Dam and Haemers showed that not all Smith graphs are determined by the spectra [23]. In this section, we show that all Smith graphs are determined by the high-order spectra.

Figure 1 shows all the Smith graphs. Except for the graphs $\widetilde{D}_n$ and $\widetilde{E}_6$, Smith graphs are determined by the spectra [23]. Then all Smith graphs are DHS if and only if $\widetilde{D}_n$ and $\widetilde{E}_6$ are DHS. In order to prove that $\widetilde{D}_n$ and $\widetilde{E}_6$ are DHS, we only need to give all non-isomorphic cospectral graphs of $\widetilde{D}_n$ (resp. $\widetilde{E}_6$) and then prove that these cospectral graphs are not high-order cospectral with $\widetilde{D}_n$ (resp. $\widetilde{E}_6$).



(a) P_n (b) D_n (c) E_6 (d) E_7

(e) E_8 (f) C_n (g) $\widetilde{D}_n$ (h) $\widetilde{E}_6$

(i) $\widetilde{E}_7$ (j) $\widetilde{E}_8$

Figure 1: Smith graphs

The following cospectral invariant of graphs in terms of the number of subgraphs was given by Cvetković and Rowlinson in [7].

Lemma 3.1. *[7] If graphs G and G^* are cospectral, then* $N_G(P_3) + 2N_G(C_4) = N_{G^*}(P_3) + 2N_{G^*}(C_4)$.

We give all non-isomorphic cospectral graphs of $\widetilde{D}_n$ (resp. $\widetilde{E}_6$) by the above cospectral invariant. Let $G_1 + G_2$ denote the disjoint union of graphs G_1 and G_2.

Lemma 3.2. *Graph G is a non-isomorphic cospectral graphs of $\widetilde{D}_n$ (resp. $\widetilde{E}_6$) if and only if $G = C_4 + P_n$ (resp. $C_6 + K_1$).*

Proof. It is well-known that $C_4 + P_n$ is a non-isomorphic cospectral graphs of $\widetilde{D}_n$ [9, Page 77]. Let G be a non-isomorphic cospectral graph of $\widetilde{D}_n$. We will show that $G = C_4 + P_n$.

Claim 1: G has two connected components, one is a cycle and the other is a tree.

Proof: Since G is cospectral with $\widetilde{D}_n$, the spectral radius of G is equal to 2. All Smith graphs are determined by the spectra, except for the graphs $\widetilde{D}_n$ and $\widetilde{E}_6$ [23]. Then G is not a Smith graph, i.e., G is not connected.

The spectral radii of every connected components of G are at most 2. Since connected graphs with spectral radii at most 2 are cycles or trees, every connected components of G are cycles or trees. From $|V(G)| = |V(\widetilde{D}_n)| = n+4$ and $|E(G)| = |E(\widetilde{D}_n)| = n+3$, we get $|E(G)| = |V(G)|-1$. Then we know that only one connected component of G is a tree and the other connected components are cycles.

The algebraic multiplicity of the eigenvalue $\lambda = 2$ of G (or $\widetilde{D}_n$) is 1 [9, Page 77], it yields that only one connected component of G is cycle and the spectral radii of the other connected components are less than 2. Then the graph G contains exactly two connected components, one of them is a cycle and the other is a tree with spectral radius less than 2. $\square$

<u>Claim 2</u>: $G = C_4 + P_n$.

<u>Proof:</u> From the proof of Claim 1, we have $G = C_s + T_{n+4-s}$, where C_s is a cycle with s vertices and T_{n+4-s} is a tree whose spectral radius is less than 2. Since G is cospectral with $\widetilde{D}_n$, we have $N_G(P_3) + 2N_G(C_4) = N_{\widetilde{D}_n}(P_3) + 2N_{\widetilde{D}_n}(C_4)$ by Lemma 3.1. We know that $N_{\widetilde{D}_n}(P_3) + 2N_{\widetilde{D}_n}(C_4) = n + 4$ from Figure 1 (g). Then

$$N_{C_s}(P_3) + N_{T_{n+4-s}}(P_3) + 2N_{C_s}(C_4) + 2N_{T_{n+4-s}}(C_4) = n + 4.$$

We have

$$\begin{aligned} 2N_{C_s}(C_4) &= n + 4 - N_{C_s}(P_3) - N_{T_{n+4-s}}(P_3) \\ &= n + 4 - s - N_{T_{n+4-s}}(P_3). \end{aligned} \tag{3.1}$$

Since the spectral radius of T_{n+4-s} is less than 2, we know that T_{n+4-s} is isomorphic to one of P_{n+4-s}, D_{n+2-n}, E_6, E_7 or E_8.

If $T_{n+4-s} = P_{n+4-s}$, we have $N_{T_{n+4-s}}(P_3) = n + 2 - s$ when $n + 4 - s \geq 3$ and $N_{T_{n+4-s}}(P_3) = 0$ when $1 \leq n - s + 4 < 3$. When $n + 4 - s \geq 3$, we have $N_{C_s}(C_4) = 1$ by Equation (3.1), i.e., $s = 4$. When $1 \leq n - s + 4 < 3$, we have $1 \leq 2N_{C_s}(C_4) < 3$ and then $N_{C_s}(C_4) = 1$ by Equation (3.1), i.e., $s = 4$. So we have $N_G(C_4) = 1$ if $T_{n+4-s} = P_{n+4-s}$.

If T_{n+4-s} is isomorphic to one of D_{n+2}, E_6, E_7 and E_8, it yields that $N_{T_{n+4-s}}(P_3) = n+3-s$ from Figure 1 (b), (c), (d) and (e). Then we get $2N_{C_s}(C_4) = 1$ by Equation (3.1). It contradicts the fact that $2N_{C_s}(C_4)$ is even.

Then we get that $G = C_4 + P_n$. $\square$

From the above proof, we know that G is a non-isomorphic cospectral graphs of $\widetilde{D}_n$ if and only if $G = C_4 + P_n$. Similarly, we also obtain that G is a non-isomorphic cospectral graphs of $\widetilde{E}_6$ if and only if $G = C_6 + K_1$. $\square$

Next, we will show that $\widetilde{D}_n^{(k)}$ (resp. $\widetilde{E}_6^{(k)}$) is not high-order cospectral with their cospectral graphs $(C_4 + P_n)^{(k)}$ (resp. $(C_6 + K_1)^{(k)}$). We show that there is an eigenvalue λ of the power hypergraph $\widetilde{D}_n^{(k)}$ (resp. $\widetilde{E}_6^{(k)}$) but λ is not an eigenvalue of $(C_4 + P_n)^{(k)}$ (resp. $(C_6 + K_1)^{(k)}$). Therefore, we obtain the main result in this section.

Theorem 3.3. *All Smith graphs are determined by the high-order spectra.*

Proof. We will prove that $\widetilde{D}_n$ and $\widetilde{E}_6$ are DHS. By Lemma 3.2, we know that graph G is a non-isomorphic cospectral graphs of $\widetilde{D}_n$ (resp. $\widetilde{E}_6$) if and only if $G = C_4 + P_n$ (resp. $C_6 + K_1$). Then we only need to prove that $\widetilde{D}_n$ (resp. $\widetilde{E}_6$) is not high-order cospectral with $(C_4 + P_n)$ (resp. $C_6 + K_1$).

Next, we prove that there is an eigenvalue λ of the hypergraph $\widetilde{D}_n^{(k)}$ such that λ is not an eigenvalue of the hypergraph $(C_4+P_n)^{(k)}$. Since D_n is an induced subgraph of $\widetilde{D}_n$ and $2\cos\frac{\pi}{2n+2}$ is an eigenvalue of D_n [9, Page 77], we know that $\sqrt[k]{(2\cos\frac{\pi}{2n+2})^2}$ is an eigenvalue of $\widetilde{D}_n^{(k)}$ from Lemma 2.1. By Lemmas 2.2 and 2.3, the largest real eigenvalue less than $\sqrt[k]{4}$ of $(C_4 + P_{n-3})^{(k)}$ is $\sqrt[k]{(2\cos\frac{\pi}{n})^2}$. From the monotonicity of the cosine function on interval $[0, \pi]$, we have $\sqrt[k]{(2\cos\frac{\pi}{2n+2})^2} > \sqrt[k]{(2\cos\frac{\pi}{n})^2}$. It follows that $\sqrt[k]{(2\cos\frac{\pi}{2n+2})^2}$ is not an eigenvalue of $(C_4 + P_{n-3})^{(k)}$. Then $\widetilde{D}_n$ is DHS.

Similarly, since D_3 is an induced subgraph of $\widetilde{E}_6$ and $2\cos\frac{\pi}{8}$ is an eigenvalue of D_3, it yields that $\sqrt[k]{(2\cos\frac{\pi}{8})^2}$ is an eigenvalue of $\widetilde{E}_6^{(k)}$ by Lemma 2.1. The largest real eigenvalue less than $\sqrt[k]{4}$ of $(C_6 + K_1)^{(k)}$ is $\sqrt[k]{(2\cos\frac{\pi}{6})^2}$. We know that $\sqrt[k]{(2\cos\frac{\pi}{8})^2}$ is not an eigenvalue of $(C_6 + K_1)^{(k)}$ by Lemma 2.3. Then $\widetilde{E}_6$ is DHS. □

4. High-order cospectral invariants of trees

In 1973, Schwenk gave a useful method to construct non-isomorphic cospectral trees and proved his famous conclusion:"Almost all trees are not DS" [20]. The cospectral trees constructed by Schwenk's method cannot be distinguished by the spectra. In this section, we give some high-order cospectral invariants of trees and our results show that there are infinitely many pairs of cospectral trees constructed by Schwenk's method can be distinguished by the high-order spectra.

Let T and T^* be two high-order cospectral trees. Then $\mathrm{S}_d(T^{(k)}) = \mathrm{S}_d(T^{*(k)})$ for all positive integers k and d. Let $\mathfrak{T}(m)$ denote the set of trees with m edges. From the spectral moment formula shown in Lemma 2.5, we obtain

$$\sum_{m=1}^{\frac{d}{k}} \frac{1}{2}(k-1)^{(|E(T)|-m)(k-1)} k^{m(k-2)+1} \sum_{\widehat{T}\in\mathfrak{T}(m)} c_{\frac{2d}{k}}(\widehat{T}) \left(N_T(\widehat{T}) - N_{T^*}(\widehat{T})\right) = 0 \quad (4.1)$$

for all positive integers $k \geq 2$. From Equation (4.1), we obtain some high-order cospectral invariants of trees.

Theorem 4.1. *If a tree T is high-order cospectral with tree T^*, then*

$$\sum_{\widehat{T}\in\mathfrak{T}(m)} c_d(\widehat{T})N_T(\widehat{T}) = \sum_{\widehat{T}\in\mathfrak{T}(m)} c_d(\widehat{T})N_{T^*}(\widehat{T}),$$

where for all positive integers d and m such that $1 \le m \le \frac{d}{2}$.

Proof. Since T and T^* are high-order cospectral, we have $\mathrm{S}_d(T^{(k)}) = \mathrm{S}_d(T^{*(k)})$ for all positive integers $k \ge 2$. Since $\mathrm{S}_d(T^{(k)}) = 0$ if $k \nmid d$, we assume $k \mid d$ in the following proof.

Let $d = kz$. From Equation (4.1), we have

$$\sum_{m=1}^{z} \frac{1}{2}(k-1)^{(|E(T)|-m)(k-1)} k^{m(k-2)+1} \sum_{\widehat{T}\in\mathfrak{T}(m)} c_{2z}(\widehat{T}) \left(N_T(\widehat{T}) - N_{T^*}(\widehat{T})\right) = 0 \qquad (4.2)$$

for all positive integers k. Let $f_m(k) = \frac{1}{2}(k-1)^{(|E(T)|-m)(k-1)} k^{m(k-2)+1}$. Let $y_m = \sum_{\widehat{T}\in\mathfrak{T}(m)} c_{2z}(\widehat{T}) \left(N_T(\widehat{T}) - N_{T^*}(\widehat{T})\right)$ for all $m \in [z]$. From Equation (4.2), we have $\sum_{m=1}^{z} f_m(k) y_m = 0$. Since $\frac{f_i(k)}{f_{i-1}(k)} = \frac{k^{k-2}}{(k-1)^{k-1}}$ for $i = 2, 3, \cdots, z$, we get $f_m(k) = f_1(k)(\frac{k^{k-2}}{(k-1)^{k-1}})^{m-1}$. Then $\sum_{m=1}^{z} f_1(k)(\frac{k^{k-2}}{(k-1)^{k-1}})^{m-1} y_m = 0$. For $z \ge 1$, let $k_i, 1 \le i \le z$ be any integers so that $0 < k_1 < \cdots < k_z$. It follows that

$$\begin{bmatrix} f_1(k_1) & f_1(k_1)\frac{k_1^{k_1-2}}{(k_1-1)^{k_1-1}} & \cdots & f_1(k_1)(\frac{k_1^{k_1-2}}{(k_1-1)^{k_1-1}})^{z-1} \\ f_1(k_2) & f_1(k_2)\frac{k_2^{k_2-2}}{(k_2-1)^{k_2-1}} & \cdots & f_1(k_2)(\frac{k_2^{k_2-2}}{(k_2-1)^{k_2-1}})^{z-1} \\ \vdots & \vdots & \vdots & \vdots \\ f_1(k_z) & f_1(k_z)\frac{k_z^{k_z-2}}{(k_z-1)^{k_z-1}} & \cdots & f_1(k_z)(\frac{k_z^{k_z-2}}{(k_z-1)^{k_z-1}})^{z-1} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_z \end{bmatrix} = 0. \qquad (4.3)$$

Then the coefficient matrix of the Equation (4.3) is a Vandermonde matrix. Since $k_1, k_2, \ldots, k_z$ are distinct, the determinant of the coefficient matrix are not equal to zero. Then $y_m = 0$ for all $m \in [z]$. □

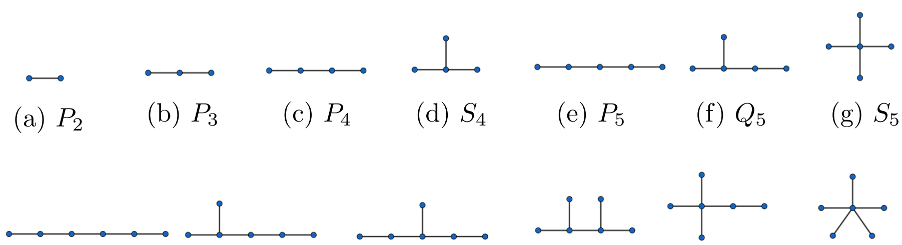
Let $m = |E(T)| = |E(T^*)|$ in Theorem 4.1, we directly get the following high-order cospectral invariants.

Theorem 4.2. *Let T and T^* be two high-order cospectral trees. Then $c_d(T) = c_d(T^*)$ for $d \ge 2|E(T)|$.*

Let $\mathfrak{T}(m) = \{\widehat{T}_1, \widehat{T}_2, \ldots, \widehat{T}_{|\mathfrak{T}(m)|}\}$. From Theorem 4.1, we get the following equation after taking d to be $d_1, d_2, \ldots, d_{|\mathfrak{T}(m)|}$.

$$\begin{bmatrix} c_{d_1}(\widehat{T}_1) & c_{d_1}(\widehat{T}_2) & \cdots & c_{d_1}(\widehat{T}_{|\mathfrak{T}(m)|}) \\ c_{d_2}(\widehat{T}_1) & c_{d_2}(\widehat{T}_2) & \cdots & c_{d_2}(\widehat{T}_{|\mathfrak{T}(m)|}) \\ \vdots & \vdots & \ddots & \vdots \\ c_{d_{|\mathfrak{T}(m)|}}(\widehat{T}_1) & c_{d_{|\mathfrak{T}(m)|}}(\widehat{T}_2) & \cdots & c_{d_{|\mathfrak{T}(m)|}}(\widehat{T}_{|\mathfrak{T}(m)|}) \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_{|\mathfrak{T}(m)|} \end{bmatrix} = 0, \tag{4.4}$$

where $h_i = N_T(\widehat{T}_i) - N_{T^*}(\widehat{T}_i)$ for all $i \in [|\mathfrak{T}(m)|]$. If there exist $d_1, d_2, \ldots, d_{|\mathfrak{T}(m)|}$ such that the coefficient matrix of Equation (4.4) is nonsingular, we get $N_T(\widehat{T}) = N_{T^*}(\widehat{T})$ for all $\widehat{T} \in \mathfrak{T}(m)$. By the formula for the spectral moment coefficients for trees, i.e. Equation (2.1), we can calculate the spectral moment coefficients $c_d(\widehat{T})$. We show the d-th order spectral moment coefficients of trees with 3 edges for $d = 6, 8$, the t-th order spectral moment coefficients of trees with 4 edges for $t = 8, 10, 12$ and the l-th order spectral moment coefficients of trees with 5 edges for $l = 10, 12, 14, 16, 18, 20$ (see Table 1 and Table 2).



(a) P_2 (b) P_3 (c) P_4 (d) S_4 (e) P_5 (f) Q_5 (g) S_5

(h) P_6 (i) Q_6 (j) R_6 (k) H_6 (l) J_6 (m) S_6

Figure 2: Trees with edges at most 5

	$c_d(P_4)$	$c_d(S_4)$
$d = 6$	6	12
$d = 8$	32	72

(a) The spectral moment coefficients of trees with 3 edges

	$c_d(P_5)$	$c_d(Q_5)$	$c_d(S_5)$
$d = 8$	8	16	48
$d = 10$	60	140	480
$d = 12$	300	804	3120

(b) The spectral moment coefficients of trees with 4 edges

Table 1: The spectral moment coefficients of trees with 3 or 4 edges

	$c_d(P_6)$	$c_d(Q_6)$	$c_d(R_6)$	$c_d(H_6)$	$c_d(J_6)$	$c_d(S_6)$
$d = 10$	10	20	20	40	60	240
$d = 12$	96	216	228	504	792	3600
$d = 14$	588	1484	1652	3976	6552	33600
$d = 16$	2944	8304	9728	25216	43680	252000
$d = 18$	13158	41328	50832	140832	257184	1668240
$d = 20$	54730	190800	245880	724320	1398600	10206000

Table 2: The spectral moment coefficients of trees with 5 edges

We obtain the following high-order cospectral invariants of trees about the number of subtrees, we can apply this result to distinguish some non-isomorphic trees.

Theorem 4.3. *If a tree T is high-order cospectral with a tree T^*, then $\widehat{T}$ is a subtree of T if and only if $\widehat{T}$ is a subtree of T^*, and $N_T(\widehat{T}) = N_{T^*}(\widehat{T})$ for any tree $\widehat{T}$ with at most 5 edges.*

Proof. Since T and T^* are high-order cospectral, we know that T and T^* are cospectral. Then $N_T(P_2) = N_{T^*}(P_2)$ and $N_T(P_3) = N_{T^*}(P_3)$ by Lemma 3.1. From Table 1 and Table 2, we get the coefficient matrix of Equation (4.4) when $m = 3, 4, 5$. It is easy to check that these coefficient matrices are nonsingular. Then $N_T(\widehat{T}) = N_{T^*}(\widehat{T})$ for all $\widehat{T} \in \mathfrak{T}(m)$, $m = 1, 2, 3, 4, 5$. Without loss of generality, let $N_T(\widehat{T}) \neq 0$, i.e, $\widehat{T}$ is a subtree of T. Then we know that $\widehat{T}$ is a subtree of T if and only if $\widehat{T}$ is a subtree of T^* and $N_T(\widehat{T}) = N_{T^*}(\widehat{T})$. □

By the above high-order cospectral invariants, we get infinitely many pairs of cospectral trees with different high-order spectra. As shown in Figure 3 and 4, let T_u and T_v be the tree T rooted at vertices u and v, respectively. For any rooted tree F, the coalescences $F \cdot T_u$ and $F \cdot T_v$, as shown in Figure 4, are cospectral trees [22].

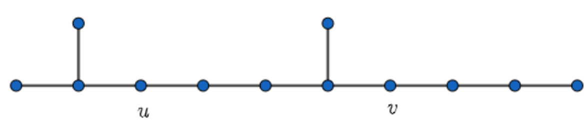
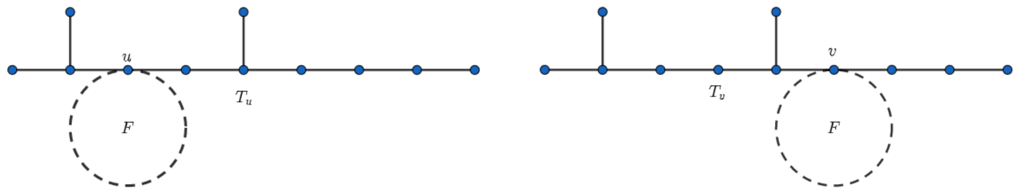


Figure 3: Tree T



(a) $F \cdot T_u$ (b) $F \cdot T_v$

Figure 4: The coalescences $F \cdot T_u$ and $F \cdot T_v$

Theorem 4.4. *Cospectral trees $F \cdot T_u$ and $F \cdot T_v$ have different high-order spectra.*

Proof. Recall that R_6 denotes the tree in Figure 2 (j). We consider the difference between the number of subgraphs of $F \cdot T_v$ and $F \cdot T_u$ that are isomorphic to R_6. Let V_0 (or U_0) denote the number of subgraphs in $F \cdot T_v$ (or $F \cdot T_u$) that are isomorphic to R_6 and do not contain the vertex v (or u).

Let V_i (or U_i) denote the number of subgraphs in $F \cdot T_v$ (or $F \cdot T_u$) that are isomorphic to R_6 and the vertex v (or u) has a degree i for $i = 1, 2, 3$. It implies that $N_{F \cdot T_v}(R_6) = \sum_{i=0}^{3} \mathrm{V}_i$ and $N_{F \cdot T_u}(R_6) = \sum_{i=0}^{3} \mathrm{U}_i$. When $i = 0$ or $i = 3$, it is easy to check that $\mathrm{V}_i = \mathrm{U}_i$ from Figure 4. When $i = 1$, we have $\mathrm{V}_1 = \mathrm{U}_1 - 1$ from Figure 4. Let d be the degree of the root of F. When $i = 2$, we have $\mathrm{V}_2 = \mathrm{U}_2 + d + 1$. Then we have $N_{F \cdot T_v}(R_6) - N_{F \cdot T_u}(R_6) = \sum_{i=0}^{3} \mathrm{V}_i - \sum_{i=0}^{3} \mathrm{U}_i = d$.

Note that R_6 is a tree with five edges. By Theorem 4.3, we know that $F \cdot T_u$ is not high-order cospectral with $F \cdot T_v$.

□

In this paper, we show that all Smith graphs are determined by the high-order spectra. And the infinitely many pairs of non-isomorphic cospectral trees constructed by Schwenk's method have different the high-order spectra. At the end of this paper, we propose the following conjecture.

Conjecture 4.5. *Two trees are isomorphic if and only if they have the same high-order spectra.*

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References

[1] Romain Boulet and Bertrand Jouve. The lollipop graph is determined by its spectrum. *Electronic Journal of Combinatorics*, 15(1):1948–1953, 2008.

[2] Lixiang Chen and Changjiang Bu. A reduction formula for the characteristic polynomial of hypergraph with pendant edges. *Linear Algebra and its Applications*, 611:171–186, 2021.

[3] Lixiang Chen, Changjiang Bu, and Jiang Zhou. Spectral moments of hypertrees and their applications. *Linear and Multilinear Algebra*, 2021. Doi:10.1080/03081087.2021.1953431.

[4] Lixiang Chen, Edwin R. van Dam, and Changjiang Bu. All eigenvalues of the power hypergraph and signed subgraphs of a graph. *Linear Algebra and its Applications*, 676:205–210, 2023.

[5] Gregory J. Clark and Joshua N. Cooper. A Harary-Sachs theorem for hypergraphs. *Journal of Combinatorial Theory, Series B*, 149:1–15, 2021.

[6] Joshua Cooper and Aaron Dutle. Spectra of uniform hypergraphs. *Linear Algebra and its Applications*, 436(9):3268–3292, 2012.

[7] Dragoš Cvetković and Peter Rowlinson. Spectra of unicyclic graphs. *Graphs and Combinatorics*, 3(1):7–23, 1987.

[8] Dragoš M. Cvetković. Graphs and their spectra. *Publikacije Elektrotehničkog fakulteta. Serija Matematika i fizika*, (354-356):1–50, 1971.

[9] Dragoš M. Cvetković, Horst Sachs, and Michael Doob. *Spectra of Graphs: Theory and Applications*. VEB Deutscher Verlag der Wissenschaften, 1980.

[10] Yi-Zheng Fan, Tao Huang, Yan-Hong Bao, Chen-Lu Zhuan-Sun, and Ya-Ping Li. The spectral symmetry of weakly irreducible nonnegative tensors and connected hypergraphs. *Transactions of the American Mathematical Society*, 372(3):2213–2233, 2019.

[11] Yi-Zheng Fan, Yue Wang, and Yi Wang. A note on the nullity of unicyclic signed graphs. *Linear Algebra and Its Applications*, 438(3):1193–1200, 2013.

[12] Chris D. Godsil and Brendan D. McKay. Constructing cospectral graphs. *Aequationes Mathematicae*, 25(1):257–268, 1982.

[13] Hs H. Günthard and Hans Primas. Zusammenhang von graphentheorie und motheorie von molekeln mit systemen konjugierter bindungen. *Helvetica Chimica Acta*, 39(6):1645–1653, 1956.

[14] Shenglong Hu, Liqun Qi, and Jiayu Shao. Cored hypergraphs, power hypergraphs and their laplacian H-eigenvalues. *Linear Algebra and its Applications*, 439:2980–2998, 2013.

[15] Mirko Lepović and Ivan Gutman. No starlike trees are cospectral. *Discrete Mathematics*, 242(1-3):291–295, 2002.

[16] Lek-Heng Lim. Singular values and eigenvalues of tensors: a variational approach. In *1st IEEE International Workshop on Computational Advances in Multi-Sensor Adaptive Processing*, pages 129–132. IEEE, 2005.

[17] Brendan D McKay. On the spectral characterisation of trees. *Ars Combinatoria*, 3:219–232, 1977.

[18] Russell Merris. Laplacian matrices of graphs: a survey. *Linear Algebra and its Applications*, 197:143–176, 1994.

[19] Liqun Qi. Eigenvalues of a real supersymmetric tensor. *Journal of Symbolic Computation*, 40(6):1302–1324, 2005.

[20] Allen J. Schwenk. Almost all trees are cospectral. In Frank Harry, editor, *New Directions in the Theory of Graphs*, pages 275–307, New York, 1973. Academic Press.

[21] John H. Smith. Some properties of the spectrum of a graph. *Combinatorial Structures and their Applications*, pages 403–406, 1970.

[22] Edwin R. van Dam and Willem H. Haemers. Which graphs are determined by their spectrum? *Linear Algebra and its Applications*, 373:241–272, 2003.

[23] Edwin R. van Dam and Willem H. Haemers. Developments on spectral characterizations of graphs. *Discrete Mathematics*, 309(3):576–586, 2009.

[24] Lothar von Collatz and Ulrich Sinogowitz. Spektren endlicher grafen. *Abhandlungen aus dem Mathematischen Seminar der Universität Hamburg*, 21(1):63–77, 1957.

[25] Wang Wei. A simple arithmetic criterion for graphs being determined by their generalized spectra. *Journal of Combinatorial Theory, Series B*, 122:438–451, 2017.

[26] Pepijn Wissing and Edwin R. van Dam. The negative tetrahedron and the first infinite family of connected digraphs that are strongly determined by the hermitian spectrum. *Journal of Combinatorial Theory, Series A*, 173:105232, 2020.

[27] Pepijn Wissing and Edwin R. van Dam. Spectral fundamentals and characterizations of signed directed graphs. *Journal of Combinatorial Theory, Series A*, 187:105573, 2022.