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THE WALKS AND CDC OF GRAPHS WITH THE SAME MAIN EIGENSPACE

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Abstract

The main eigenvalues of a graph G are those eigenvalues of the (0, 1)adjacency matrix \mathbf{A} with a corresponding eigenspace not orthogonal to $\mathbf{j} = (1 \mid 1 \mid \cdots \mid 1)^{\mathsf{T}}$. The principal main eigenvector associated with a main eigenvalue is the orthogonal projection of the corresponding eigenspace onto \mathbf{j} . The main eigenspace of a graph is generated by all the principal main eigenvectors and is the same as the image of the walk matrix. We explore a new concept to see to what extent the main eigenspace determines the entries of the walk matrix of a graph. The CDC of a graph G is the direct product $G \times K_2$. We establish a hierarchy of inclusions connecting classes of graphs in view of their CDC, walk matrix, main eigenvalues and main eigenspaces. We provide a new proof that graphs with the same CDC are characterized as TF-isomorphic graphs. A complete list of TF-isomorphic graphs on at most 8 vertices and their common CDC is also given.

Keywords: bipartite (canonical) double covering, main eigenspace, comain graphs, walk matrix, two-fold isomorphism.

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1. INTRODUCTION

A graph G = (V, E) of order n has a vertex set $V = \{1, \ldots, n\}$ and an edge set $E \subseteq \{\{u, v\} : u, v \in V \text{ and } u \neq v\}$. We consider graphs which are simple, that is, graphs which are undirected, without multiple edges or loops. A k-walk in a graph G is a k-tuple $(u_0, u_1, \ldots, u_k) \in V^{k+1}$ such that $\{u_{i-1}, u_i\} \in E$, for all $1 \leq i \leq k$.

Let graphs G_i , $1 \leq i \leq k$, have order n_1, n_2, \ldots, n_k , respectively. The disjoint union of the graphs G_i , denoted by $G_1 \cup \cdots \cup G_k$ or $\bigcup_{i=1}^k G_i$, is the disconnected graph of order $n_1 + n_2 + \cdots + n_k$, having the k components G_i .

The adjacency matrix of a graph G, denoted by $\mathbf{A}(G)$, or simply \mathbf{A} where the context is clear, is the symmetric $n \times n$ matrix (a_{ij}) , where $a_{ij} = 1$ if $\{i, j\} \in E$, and $a_{ij} = 0$ otherwise. We use terminology for a graph G and its adjacency matrix \mathbf{A} interchangeably, since the graph G is determined, up to relabelling of the vertices, by \mathbf{A} . Thus the eigenvalues and eigenvectors of a graph G are respectively those of the matrix \mathbf{A} . The spectrum spec(G) of a graph G is the multiset consisting of the s distinct eigenvalues μ_1, \ldots, μ_s , each occurring $m(\mu_i)$ times, $1 \leq i \leq s$, where the multiplicity $m(\mu_i)$ is the number of times that μ_i is repeated as a root of the characteristic polynomial det $(\lambda \mathbf{I} - \mathbf{A})$. Since \mathbf{A} is real-symmetric, $m(\mu_i)$ is the dimension of the eigenspace $\mathscr{C}_G(\mu_i)$ associated with μ_i , where $\mathscr{C}_G(\mu_i) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{A}\mathbf{x} = \mu_i \mathbf{x}\}$.

Two graphs G_1 and G_2 are isomorphic if there exists a permutation matrix \mathbf{P} such that $\mathbf{P}^{\mathsf{T}} \mathbf{A}(G_1) \mathbf{P} = \mathbf{A}(G_2)$ whereas the graphs are two-fold (TF) isomorphic if there exist permutation matrices \mathbf{P} and \mathbf{Q} such that $\mathbf{P}^{\mathsf{T}} \mathbf{A}(G_1) \mathbf{Q} = \mathbf{A}(G_2)$. Isomorphic graphs have the same underlying graph with different labellings. The adjacency matrices of isomorphic graphs are similar whereas those of TF-isomorphic graphs are congruent.

Let \boldsymbol{j} denote the vector $(1 \mid 1 \mid \dots \mid 1)^{\mathsf{T}}$. The number of distinct eigenvalues of an *n*-vertex graph is taken to be s. The eigenvalues $\mu_1, \mu_2, \dots, \mu_p$ of G $(1 \leq p \leq s \leq n)$ having an associated eigenvector \boldsymbol{x} not orthogonal to \boldsymbol{j} (that is $\langle \boldsymbol{x}, \boldsymbol{j} \rangle \neq 0$) are said to be *main*. Their eigenspace determines the number of walks of G. The remaining distinct eigenvalues $\mu_{p+1}, \mu_{p+2}, \dots, \mu_s$ are *non-main*.

Spectral decomposition of **A** yields

(1)
$$\mathbf{A} = \sum_{i=1}^{s} \mu_i \mathbf{P}_i$$

where $\mathbf{P}_i \colon \mathbb{R} \to \mathscr{C}_G(\mu_i)$ is the orthogonal projection of \mathbb{R}^n onto the eigenspace $\mathscr{C}_G(\mu_i)$ for $\mu_i, 1 \leq i \leq s$. Note that, for $1 \leq i \leq s$, the non-zero columns of \mathbf{P}_i are eigenvectors associated with the eigenvalue μ_i . For $1 \leq i \leq p$, the principal main eigenvector of μ_i is $\mathbf{P}_i \mathbf{j}$. Moreover, the sum $\sum_{i=1}^p \mathbf{P}_i \mathbf{j} = \mathbf{j}$.

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A pair of graphs G and H are *comain* if they have the same set of main eigenvalues (ignoring multiplicity). The *main eigenspace*, Main(G), is the space generated by all the principal main eigenvectors. Thus

(2)
$$\operatorname{Main}(G) = \operatorname{Span}\{\mathbf{P}_1\,\boldsymbol{j},\ldots,\mathbf{P}_p\,\boldsymbol{j}\}.$$

The entry $a_{ij}^{(k)}$ of the matrix \mathbf{A}^k is the number of walks of length k starting from vertex i and ending at vertex j. Then the *i*th entry of $\mathbf{A}^k j$ is the total number of walks of length k starting from vertex i. For i = 1, 2, ..., k, the $n \times k$ matrix, $\mathbf{W}_G(k)$, whose k columns are $\mathbf{A}^{i-1}j$ is the k-walk matrix of G

$$\mathbf{W}_{G}(k) = \left(\begin{array}{c} \boldsymbol{j} \mid \mathbf{A}\boldsymbol{j} \mid \mathbf{A}^{2}\boldsymbol{j} \mid \cdots \mid \mathbf{A}^{k-1}\boldsymbol{j} \end{array}
ight).$$

Walks and main eigenvalues are closely related. It turns out that the number of walks of length k in an *n*-vertex graph G is given by

(3)
$$N_{k} = \sum_{i=1}^{p} \left\| \mathbf{P}_{i} \mathbf{j} \right\|^{2} \mu_{i}^{k} = c_{1}^{\prime} \mu_{1}^{k} + c_{2}^{\prime} \mu_{2}^{2} + \dots + c_{p}^{\prime} \mu_{p}^{k},$$

where μ_i , for i = 1, ..., p, are the main eigenvalues of G, \mathbf{P}_i is the orthogonal projection of \mathbb{R}^n onto the eigenspace of μ_i and $c'_i = \|\mathbf{P}_i \mathbf{j}\|^2$ is the square of the length of the principal main eigenvector associated with μ_i . The constants c'_i are independent of the length k of the walk [3, p. 44].

If G has p main eigenvalues, then the rank of the walk matrix $\mathbf{W}_G(k)$ with k columns is min $\{k, p\}$ [9]. It follows that the first p columns of $\mathbf{W}_G(k)$ are linearly independent and form a basis for the column space of $\mathbf{W}_G(k)$. Therefore we can restrict the number of columns of the walk matrix of a graph.

Definition 1. The walk matrix \mathbf{W}_G (or \mathbf{W}) of a graph G having p distinct main eigenvalues is the p-walk matrix $\mathbf{W}_G(p)$ of G.

It is the purpose of this article to use the *canonical double covering* (also referred to as *bipartite double covering* in the literature) of a graph to investigate the relation between the walk matrix and the main eigenspace.

The canonical double covering, CDC(G), of a graph G = (V, E) of order n, is a graph G' = (V', E') of order 2n where $V' = V \times \{0, 1\}$, and

$$E' = \{\{(u,0), (v,1)\}, \{(u,1), (v,0)\} : \{u,v\} \in E\}.$$

In other words, CDC(G) is obtained by producing two copies of the vertex set, and replacing edges $\{u, v\}$ in the original graph by edges from the first copy to the second copy, and vice versa. It is always bipartite, with partite sets $V \times \{0\}$ and $V \times \{1\}$. The CDC of the 3-cycle C_3 is the 6-cycle C_6 . Figure 1 shows the CDC of the complete bipartite graph $K_{2,3}$.

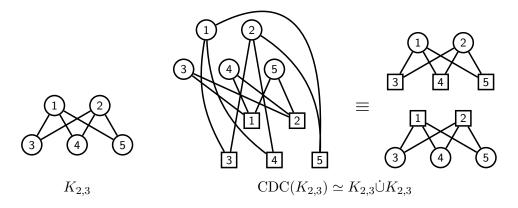


Figure 1. Canonical double coverings of $K_{2,3}$, where vertices (v, 0) are represented by circle nodes, and vertices (v, 1) by square nodes.

It is well known that the main eigenspace is the same as the column space of the walk matrix [11]. This prompts the question.

How are the walk matrices of non-isomorphic graphs with the same main eigenspace related?

This is investigated in Section 2. We show that there is a close relationship, even when the graphs are not comain. In Section 2, we also show that non-isomorphic graphs with the same CDC have the same walk matrix and that the converse is false.

We determine minimal conditions that ensure that graphs share the same k-walk matrix, in Section 3. When comain graphs share the same walk matrix $W(:=W_p)$, then for both graphs W can be extended to the same W_k for $k \ge p$. For $p \geq 2$, graphs with the same W have the same degree sequence. We also focus on the specific principal main eigenvectors and the main eigenspace. We show that graphs with the same main eigenspace that are not comain have a different degree sequence. There has been a great interest, recently, in the research on walks in graphs [7]. In this paper, graphs with the same CDC are proved to have the same walk matrix and we show that the converse is false. A pair of graphs on 6 vertices with the same main eigenspace, has appeared in the literature as a pair of graphs that have the same CDC [12]. This pair of graphs, which we call the Zelinka pair, was the basis of a study on TF-isomorphic graphs [6]. In Section 4, we give a new proof of the characterization of TF-isomorphic graphs as the graphs sharing the same CDC. In this study related classes of graphs have been identified. In Section 5, we establish a hierarchy of inclusions, connecting the different classes of graphs in view of their CDC, walk matrix, main eigenvalues

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and main eigenspaces. This is illustrated in a relation diagram given in Figure 7. Furthermore, in Appendix, to supplement the Zelinka pair of graphs, we give an exhaustive list of all pairs of TF-isomorphic graphs on at most 8 vertices and their corresponding CDC.

2. The Canonical Double Covering and the Walk Matrix

Let V 0 be the vertex set of : : : on n vertices. So, V 0 = : : : etc.; Page 5.

Let V' be the vertex set of CDC(G) of a graph G = (V, E) on n vertices. The set V' can be expressed as $V \times \{0, 1\}$. The vertex labelling of CDC(G) assigns the first n labels to the n vertices in $\mathcal{V} \times \{0\}$, followed by the labelling (in the same order) of $\mathcal{V} \times \{1\}$. For this labelling, the adjacency matrix of CDC(G) is given by

$$\mathbf{A}(\mathrm{CDC}(G)) = \left(\begin{array}{c|c} \mathbf{O} & \mathbf{A}(G) \\ \hline \mathbf{A}(G) & \mathbf{O} \end{array}\right).$$

This is equivalent to the direct product of G with K_2 , that is $\text{CDC}(G) = G \times K_2$. It can also be obtained as the NEPS of G and K_2 with basis $\{(1,1)\}$ [3]. Consequently, the eigenvalues of CDC(G) are those of G and their negatives; that is μ is an eigenvalue of G with multiplicity η if and only if $\pm \mu$ are eigenvalues of CDC(G) with the same multiplicity η [3].

The CDC is bipartite and distinguishes between bipartite and non-bipartite connected graphs. A connected graph G is bipartite if and only if CDC(G) is disconnected. If G is bipartite, then $\text{CDC}(G) \simeq G \dot{\cup} G$. Figure 1 shows the CDC of the bipartite graph $K_{2,3}$. Moreover the CDC operation is additive with respect to disjoint union. If $G = G_1 \dot{\cup} \cdots \dot{\cup} G_k$ and G_i is connected for $1 \leq i \leq k$, then

$$\operatorname{CDC}(G) = \operatorname{CDC}\left(\bigcup_{i=1}^{k} G_i\right) \simeq \bigcup_{i=1}^{k} \operatorname{CDC}(G_i).$$

A remarkable property of graphs, that share the same labelled CDC, is that the number of walks of any length from corresponding vertices in the respective graphs is the same.

Theorem 2. Let G, H be two labelled graphs with $\text{CDC}(G) \simeq \text{CDC}(H)$. Let k be a natural number. Then

$$\mathbf{W}_G(k) = \mathbf{W}_H(k)$$

for appropriate labelling of the vertices.

Proof. To simplify notation, for a graph Γ , we write \mathbf{A}_{Γ} and \mathbf{C}_{Γ} (or \mathbf{C}) for $\mathbf{A}(\Gamma)$ and $\mathbf{A}(\text{CDC}(\Gamma))$, respectively. Since $\text{CDC}(G) \simeq \text{CDC}(H)$, we can relabel

the vertices of the graph H so that $\mathbf{C}_G = \mathbf{C}_H$. Now, for all ℓ , $0 \leq \ell \leq k$, the $(\ell+1)$ th column of the walk matrix of \mathbf{C}_G and \mathbf{C}_H will be the 2×1 block matrices

$$\mathbf{C}_{\mathbf{G}}{}^{\ell}\boldsymbol{j} = \left(rac{\mathbf{A}_{G}{}^{\ell}\boldsymbol{j}}{\mathbf{A}_{G}{}^{\ell}\boldsymbol{j}}
ight) \qquad ext{and} \qquad \mathbf{C}_{H}{}^{\ell}\boldsymbol{j} = \left(rac{\mathbf{A}_{H}{}^{\ell}\boldsymbol{j}}{\mathbf{A}_{H}{}^{\ell}\boldsymbol{j}}
ight),$$

respectively, but since $\mathbf{C}_G = \mathbf{C}_H$, it follows that $\mathbf{A}_G^{\ell} \mathbf{j} = \mathbf{A}_H^{\ell} \mathbf{j}$ for all $\ell, 0 \leq \ell \leq k$. It follows that the columns of $\mathbf{W}_G(k)$ and $\mathbf{W}_H(k)$ are equal.

The converse of Theorem 2 is false.

Counterexample 3. A counterexample establishing that the converse of Theorem 2 is false is given by the graphs illustrated in Figure 2. Indeed, these graphs have (1 - 2 - 0)

$$\mathbf{W}_{G} = \begin{pmatrix} 1 & 3 & 9 \\ 1 & 3 & 10 \\ 1 & 3 & 10 \\ 1 & 3 & 10 \\ 1 & 3 & 10 \\ 1 & 3 & 9 \\ 1 & 4 & 12 \end{pmatrix} = \mathbf{W}_{H},$$

but $CDC(G) \simeq CDC(H)$.

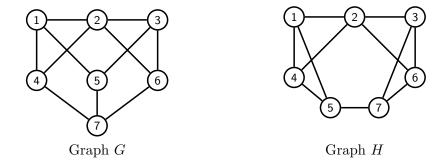


Figure 2. The graphs G and H have the same walk matrix but different CDC.

3. The Walk Matrix and Main Eigenspace

In [11], the column space of $\mathbf{W}_G(k)$ is shown to be the same as the subspace Main(G). For main eigenvalues μ_1, \ldots, μ_p of G, according to [4], the main characteristic polynomial $M(G, x) = \prod_{i=1}^{p} (x - \mu_i) = x^p - c_0 x^{p-1} - \cdots - c_{p-2} x - c_{p-1}$. The next result presents minimal conditions for two graphs to have the same k-walk matrix.

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Theorem 4. Let two comain graphs have p main eigenvalues and the same walk matrix. Then W can be extended to the same k-walk matrix for any $k \ge p$.

Proof. Let G and H be two comain graphs with the same walk matrix W. Since $\mathbf{P}_i \mathbf{j}$ is an eigenvector associated with μ_i , then for $1 \leq i \leq p$, $(\mathbf{A} - \mu_i \mathbf{I}) \mathbf{P}_i \mathbf{j} = \mathbf{0}$. Therefore $M(G, x)\mathbf{j} = \prod_{i=1}^{p} (\mathbf{A} - \mu_i \mathbf{I}) \sum_{j=1}^{p} \mathbf{P}_j \mathbf{j} = \mathbf{0}$ [10]. It follows that $(\mathbf{A})^p \mathbf{j} - c_0(\mathbf{A})^{p-1} \mathbf{j} - \cdots - c_{p-2} \mathbf{A} \mathbf{j} - c_{p-1} \mathbf{I} \mathbf{j} = 0$, which provides a recurrence relation for the kth column of $\mathbf{W}_G(k)$ as a linear combination of the previous p columns, for $k \geq p$. Observe that the coefficients of the main characteristic polynomial and the first p columns of the walk matrix are the same for both graphs. Hence the kth column of $\mathbf{W}_G(k)$ is the same as the the j-th column of $\mathbf{W}_H(k)$ for all $j, 0 \leq j \leq k$.

Theorem 4 shows that minimal conditions for two graphs to have a common k-walk matrix for any $k \in \mathbb{Z}^+$ are that they have the same main eigenvalues and the same \mathbf{W} . Since the entries of the companion matrix \mathbf{Q} of the main characteristic polynomial M(G, x) depend only on the main eigenvalues, graphs sharing the same \mathbf{W} and \mathbf{Q} suffice to determine the k-walk matrix, thus providing another set of minimal conditions for two graphs to have the same k-walk matrix.

Theorem 5. The k-walk matrix of a graph G can be expressed in terms of \mathbf{W} and the entries of \mathbf{Q} .

 $\begin{aligned} & \boldsymbol{Proof.} \text{ Let the main characteristic polynomial } M(G, x) \text{ be } M(G, x) = \prod_{i=1}^{p} (x - \mu_i) = x^p - c_0 x^{p-1} - \dots - c_{p-2} x - c_{p-1}. \\ & \text{Then the companion matrix } \mathbf{Q} \text{ is } \begin{pmatrix} 0 & 0 & \dots & 0 & c_{p-1} \\ 1 & 0 & \dots & 0 & c_{p-2} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & c_0 \end{pmatrix} \text{ and } \mathbf{AW} = \mathbf{WQ}. \\ & \text{Since } M(G, \mathbf{A}) \mathbf{j} = \mathbf{0}, \ \mathbf{A}^p \mathbf{j} = \mathbf{W} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{p-1} \end{pmatrix}. \text{ It follows that, for } 1 \leq \ell \leq k, \\ & \text{the } (p + \ell) \text{th column of } \mathbf{W}_G(k) \text{ is } A^{p+\ell-1}\mathbf{j}. \text{ For } k = (p+\ell), \text{ the } k\text{-th column of } \\ & \mathbf{W}_G(k) \text{ can be expressed as } \mathbf{WQ}^{\ell-1} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{p-1} \end{pmatrix}. \end{aligned}$

Even if the principal main eigenvectors of two n-vertex graphs are the same, the walk matrix is not uniquely determined.

Theorem 6. Non-comain non-regular graphs with the same principal main eigenvectors have a different walk matrix.

Proof. Let G and H have the same principal main eigenvectors $\{\mathbf{z}_1, \ldots, \mathbf{z}_p\}$, but different eigenvalues, μ_1^G, \ldots, μ_p^G and μ_1^H, \ldots, μ_p^H , respectively. Since the \mathbf{z}_i are projections onto distinct eigenspaces, they are mutually orthogonal and therefore linearly independent. Note that $\mathbf{z}_1 + \cdots + \mathbf{z}_p = \mathbf{j}$. Column q + 1 of $\mathbf{W}_G(k)$ is

$$\mathbf{A}_G^q \mathbf{j} = \sum_{i=1}^p \mathbf{A}_G^q \mathbf{z}_i = \sum_{i=1}^p (\mu_i^G)^q \mathbf{z}_i.$$

Similarly

$$\mathbf{A}_{H}^{q}\boldsymbol{j} = \sum_{i=1}^{p} (\mu_{i}^{H})^{q} \mathbf{z}_{i}.$$

Since the \mathbf{z}_i are linearly independent and $\{\mu_i^G\} \neq \{\mu_i^H\}$, column q of the walk matrix is different for the two graphs for $q \geq 2$.

Example 7. The graphs G and H, shown in Figure 3, satisfy the conditions of Theorem 6 and have the same principal main eigenvectors

$$\left(\frac{1}{2}(-1\pm\sqrt{5}),\frac{1}{2}(-1\pm\sqrt{5}),\frac{1}{2}(-1\pm\sqrt{5}),\frac{1}{2}(-1\pm\sqrt{5}),\frac{1}{2}(-1\pm\sqrt{5}),1,1,1,1\right).$$

Hence they have the same column space of their walk matrix \mathbf{W} . However, their walk matrices \mathbf{W} are different

$$\mathbf{W}_{G} = \begin{pmatrix} 1 & 2 \\ 1 & 2 \\ 1 & 2 \\ 1 & 2 \\ 1 & 4 \\ 1 & 4 \\ 1 & 4 \\ 1 & 4 \end{pmatrix} \quad \text{and} \quad \mathbf{W}_{H} = \begin{pmatrix} 1 & 3 \\ 1 & 3 \\ 1 & 3 \\ 1 & 3 \\ 1 & 6 \\ 1 & 6 \\ 1 & 6 \\ 1 & 6 \\ 1 & 6 \end{pmatrix}$$

Note that the two graphs are not comain. The graph G has main eigenvalues $1 \pm \sqrt{5}$, whereas H has main eigenvalues $\frac{3}{2}(1 \pm \sqrt{5})$.

It is worth stating that in Example 7, the graphs have the same main eigenvectors and therefore the same column space of their respective \mathbf{W} . Now, we verify that the conditions of Theorem 4 are minimal. The walk matrix \mathbf{W} alone is not sufficient to determine the number of walks of arbitrary length from any vertex.

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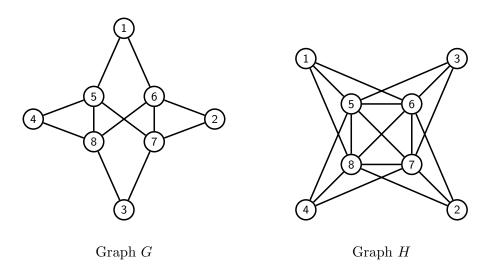


Figure 3. Graphs G and H have the same principal main eigenvectors, but have different walk matrices.

Example 8. A walk matrix $\mathbf{W}_G(p) = \mathbf{W}_H(p)$ common to two non-comain graphs G and H does not necessarily extend to the same k-walk matrix for arbitrary k > p. The two pairs $(G_{5\,622}, G_{12\,058})$ and $(G_{5\,626}, G_{12\,093})$ shown in Figures 5 and 6 are the smallest pairs (with respect to the number of vertices), obtained by a programming and computer search using Wolfram Mathematica [5]. Moreover, they are the only examples on at most 8 vertices having the same walk matrix, but not the same k-walk matrix for $k \ge p$. Throughout the article, the numbering of the graphs is in accordance with the list of non-isomorphic graphs on 8 vertices provided on Brendan McKay's graph data website [8].

Example 8 shows that having the same walk matrix is not sufficient for graphs to have the same k-walk matrix for all $k \in \mathbb{Z}^+$. Next we prove that *not* even having the same main eigenvalues suffices for two graphs to have the same k-walk matrix.

Counterexample 9. The graphs G and H of Figure 4 show that the condition that the graphs are comain does not suffice to prove that two graphs have the same k-walk matrix. Indeed, they both have main characteristic polynomial $x(x^3 - 2x^2 - 4x + 7)$, but their CDCs are not isomorphic and their walk matrices are

$$\mathbf{W}_{G} = \begin{pmatrix} 1 & 2 & 6 & 12 \\ 1 & 2 & 4 & 10 \\ 1 & 2 & 6 & 12 \\ 1 & 2 & 6 & 12 \\ 1 & 4 & 8 & 24 \\ 1 & 2 & 6 & 14 \\ 1 & 2 & 6 & 14 \end{pmatrix}, \qquad \mathbf{W}_{H} = \begin{pmatrix} 1 & 2 & 6 & 12 \\ 1 & 3 & 7 & 19 \\ 1 & 2 & 6 & 14 \\ 1 & 3 & 7 & 19 \\ 1 & 2 & 6 & 12 \\ 1 & 3 & 5 & 15 \\ 1 & 1 & 3 & 5 \end{pmatrix}.$$

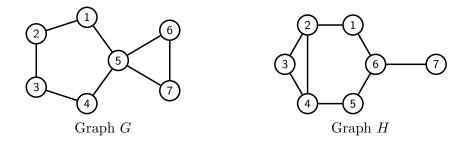


Figure 4. Graphs G and H have the same main eigenvalues, but have different walk matrices and different CDCs.

Examples 8 and 9 show that the conditions required in Theorem 4 are indeed minimal.

The walk matrix sheds light on the degree sequence of a graph. The k-walk matrix of a ρ -regular graph on n vertices is $(1 \mid \rho \mid \rho^2 \mid \cdots \mid \rho^{k-1})\mathbf{j}$ and depends only on ρ .

Theorem 10. Non-regular connected graphs with the same walk matrix have the same degree sequence.

Proof. Let G and H be non-regular connected graphs with the same walk matrix. A graph is regular if and only if it has exactly one main eigenvalue. For a connected graph with more than one main eigenvalue, the number of columns of \mathbf{W} is at least two. The second column of \mathbf{W}_G is $\mathbf{A}(\mathbf{G})\mathbf{j}$, whose entries are the vertex degrees of the labelled graph. Since $\mathbf{W}_G = \mathbf{W}_H$, the two graphs have the same degree sequence.

4. Graphs with the Same CDC and TF-Isomorphism

If two graphs G, H have isomorphic canonical double coverings, we do not necessarily have that both G and H are connected. Indeed, for instance, $\text{CDC}(C_6) \simeq \text{CDC}(K_3 \cup K_3)$. However, we do have the following lemma which will be useful in the next theorem.

Lemma 11. Let G and H be two graphs with $CDC(G) \simeq CDC(H)$. Then G has no isolated vertices if and only if H has no isolated vertices.

Proof. If G has an isolated vertex, then there exists graph G' such that $G = G' \dot{\cup} K_1$. So $\text{CDC}(G) = \text{CDC}(G' \dot{\cup} K_1) = \text{CDC}(G') \dot{\cup} \text{CDC}(K_1) = \text{CDC}(G') \dot{\cup} \overline{K_2}$ and therefore $\text{CDC}(H) = \text{CDC}(G') \dot{\cup} \overline{K_2}$. Thus the matrix

$$\mathbf{A}(\mathrm{CDC}(H)) = \left(\begin{array}{c|c} \mathbf{O} & \mathbf{A}(H) \\ \hline \mathbf{A}(H) & \mathbf{O} \end{array}\right)$$

has two zero columns, corresponding to the isolated vertices which make up $\overline{K_2}$. But a column of zeros in the matrix above arises only when a zero column is present in one of the non-zero blocks $\mathbf{A}(H)$, and since both non-zero blocks are equal to $\mathbf{A}(H)$, these two columns must be distributed equally between both blocks. This zero column of $\mathbf{A}(H)$ corresponds to an isolated vertex in H. The converse follows immediately by construction of a CDC.

The relation $\mathbf{Q}\mathbf{A}_{G}\mathbf{R} = \mathbf{A}_{H}$, where the permutation matrices \mathbf{Q} and \mathbf{R} are not inverses presents a weakened form of graph isomorphism. It is called *two-fold isomorphism* or *TF-isomorphism*, and we write $G \cong^{TF} H$ for the *TF-isomorphic* graphs G and H.

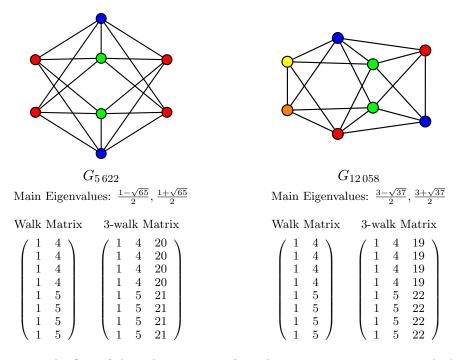


Figure 5. The first of the only two pairs of graphs on at most 8 vertices, with the same **W** (and therefore the same main eigenspace) but different $\mathbf{W}(k)$ for $k \ge 3$ as described in Example 8.

TF-isomorphism was first studied by Lauri *et al.* in [6]. They show, using a combinatorial argument that TF-isomorphic graphs are graphs with the same CDC. We present a different proof by showing that the adjacency matrices of graphs sharing the same CDC are congruent.

Theorem 12. Suppose G and H are two graphs with adjacency matrices \mathbf{A}_G and \mathbf{A}_H . Then $\text{CDC}(G) \simeq \text{CDC}(H)$ if and only if there exist two permutation

matrices \mathbf{Q} and \mathbf{R} such that

$$\mathbf{Q}\mathbf{A}_{G}\mathbf{R}=\mathbf{A}_{H}.$$

Proof. Suppose, without loss of generality, that the graphs G and H have no isolated vertices (if they do, then by Lemma 11, we could pair them off until we are left with two graphs having no isolated vertices). If $\text{CDC}(G) \simeq \text{CDC}(H)$,

then there exists a permutation matrix $\mathbf{P} = \begin{pmatrix} \mathbf{P}_{11} & \mathbf{P}_{12} \\ \mathbf{P}_{21} & \mathbf{P}_{22} \end{pmatrix}$ such that $\mathbf{P}^{\top} \begin{pmatrix} \mathbf{O} & | \mathbf{A}_G \\ \mathbf{A}_G & | \mathbf{O} \end{pmatrix} \mathbf{P} = \begin{pmatrix} \mathbf{O} & | \mathbf{A}_H \\ \mathbf{A}_H & | \mathbf{O} \end{pmatrix}$. $\mathbf{P}^{\top} \begin{pmatrix} \mathbf{O} & | \mathbf{A}_G \\ \mathbf{A}_G & | \mathbf{O} \end{pmatrix} \mathbf{P} = \begin{pmatrix} \mathbf{O} & | \mathbf{A}_H \\ \mathbf{A}_H & | \mathbf{O} \end{pmatrix}$. $\mathbf{G}_{5\,626}$ Main Eigenvalues: $1 + \sqrt{17}, 1 - \sqrt{17}$ Walk Matrix 3-walk Matrix $\begin{pmatrix} 1 & 4 \\ 1 & 4 \\ 1 & 4 \\ 1 & 4 \\ 1 & 4 \\ 1 & 6 \\ 1 & 6 \\ 1 & 6 \\ 1 & 6 \end{pmatrix} \begin{pmatrix} 1 & 4 & 24 \\ 1 & 6 & 28 \\ 1 & 6 & 2$

Figure 6. The second of the only two pairs of graphs on at most 8 vertices, with the same **W** (and therefore the same main eigenspace) but different $\mathbf{W}(k)$ for $k \ge 3$ as described in Example 8.

Since all the matrices have non-negative entries,

(4)
$$\mathbf{P}_{21}^{\top}\mathbf{A}_{G}\mathbf{P}_{12} + \mathbf{P}_{11}^{\top}\mathbf{A}_{G}\mathbf{P}_{22} = \mathbf{A}_{H},$$

(5)
$$\mathbf{P}_{21}^{\top}\mathbf{A}_{G}\mathbf{P}_{11} = \mathbf{P}_{12}^{\top}\mathbf{A}_{G}\mathbf{P}_{22} = \mathbf{O}.$$

Observe that $(\mathbf{P}_{11} + \mathbf{P}_{21})^{\top} \mathbf{A}_G(\mathbf{P}_{22} + \mathbf{P}_{12}) = \mathbf{A}_H$ by (4) and (5). Now suppose $\mathbf{Q} := (\mathbf{P}_{11} + \mathbf{P}_{21})^{\top}$ or $\mathbf{R} := \mathbf{P}_{22} + \mathbf{P}_{12}$ is not a permutation matrix. Being the

sum of two submatrices of \mathbf{P} , this can only happen if a row and a column are zero. But then \mathbf{A}_H will have a row of zeros, corresponding to an isolated vertex in H, a contradiction.

Conversely, if $\mathbf{Q}\mathbf{A}_G\mathbf{R} = \mathbf{A}_H$, then $\mathbf{P} := \begin{pmatrix} \mathbf{O} & | \mathbf{Q} \\ \hline \mathbf{R}^\top & | \mathbf{O} \end{pmatrix}$ defines a permutation matrix, and

$$\mathbf{P}^{\top} \begin{pmatrix} \mathbf{O} & \mathbf{A}_G \\ \hline \mathbf{A}_G & \mathbf{O} \end{pmatrix} \mathbf{P} = \begin{pmatrix} \mathbf{O} & \mathbf{A}_H \\ \hline \mathbf{A}_H & \mathbf{O} \end{pmatrix},$$

as required.

In [6], the authors discuss a pair of TF-isomorphic graphs on 7 vertices found by B. Zelinka. In Appendix, we present an exhaustive list of 32 non-isomorphic graph pairs on up to 8 vertices that have the same CDC. The Zelinka example corresponds to the pair (G_{1164}, H_{1032}).

5. Establishing the Hierarchy

In this section, we compare the strength of relationships and similarities among classes of graphs characterized by their main eigenvalues, main eigenspaces, principal main eigenvectors, walk matrices, and CDCs. This establishes a hierarchy of inclusions among different classes of graphs.

As seen in Figure 7, a partial order of nested classes of graphs with specific combinatorial and spectral properties can be deduced. That the set of graphs with isomorphic CDCs is a subset of graphs sharing the same walk matrix is established in Theorem 2. The converse of 2, is false and this is shown by the properties of the graphs in Example 3, which have different k-walk matrices. Being TF-isomorphic and having isomorphic CDC are equivalent and this is established by Theorem 12.

Let us consider other links among the classes of graphs being considered. In [11], the class of graphs with the same walk matrix is shown to be a subclass of graphs with the same main eigenspace. But does this mean that the principal main eigenvectors $\{\mathbf{P}_1 j, \ldots, \mathbf{P}_p j\}$ which generate the main eigenspace are the same? We show that this is not the case, in the following example.

Counterexample 13. The two pairs of graphs in Figures 5 and 6 have the same walk matrix but different principal main eigenvectors. Moreover, by Theorem 6, their k-walk matrix is different since they are not comain.

The graphs of the first pair $(G_{5\,622}, G_{12\,058})$ have the following two respective

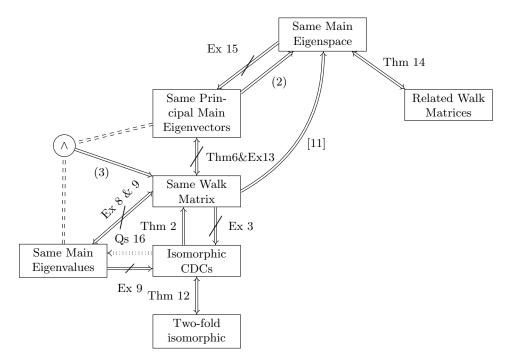


Figure 7. The hierarchy among the different classes of graphs: The symbol \Rightarrow means "implies". The dashed lines which merge at the \land node denote the conjunction of those two conditions. The dotted lines denote Question 16.

principal main eigenvectors:

$$G_{5\,622}: \quad \frac{1}{8} \left(-1 \pm \sqrt{65}, -1 \pm \sqrt{65}, -1 \pm \sqrt{65}, -1 \pm \sqrt{65}, 8, 8, 8, 8 \right),$$

$$G_{12\,058}: \quad \frac{1}{6} \left(-1 \pm \sqrt{37}, -1 \pm \sqrt{37}, -1 \pm \sqrt{37}, -1 \pm \sqrt{37}, 6, 6, 6, 6 \right).$$

The main eigenvectors corresponding to $G_{5\,622}$ are not scalar multiples of those corresponding to $G_{12\,058}$, but both separately span the same main eigenspace.

Finally we elaborate on what is meant by "related walk matrices" in Figure 7. Note that the column space of the walk matrix \mathbf{W} of graphs with the same main eigenspace is the same even when the entries of \mathbf{W} are different as shown by the graphs shown in Figure 7.

Theorem 14. Let G and H be two graphs. Then Main(G) = Main(H) if and only if there is an invertible matrix \mathbf{Q} such that $\mathbf{W}_G \mathbf{Q} = \mathbf{W}_H$.

Proof. If Main(G) = Main(H), then the column vectors of \mathbf{W}_G and \mathbf{W}_H form bases for the same space [11]. In particular, the columns of \mathbf{W}_H can be expressed

as a linear combination of those of \mathbf{W}_G . Indeed, if the *i*th column \mathbf{c}_i of \mathbf{W}_H is $\alpha_{1i}\mathbf{j} + \alpha_{2i}\mathbf{A}_G\mathbf{j} + \cdots + \alpha_{pi}(\mathbf{A}_G)^{p-1}\mathbf{j}$, then

$$\mathbf{W}_{H} = \begin{pmatrix} | & | & | \\ \mathbf{c}_{1} & \mathbf{c}_{2} & \cdots & \mathbf{c}_{p} \end{pmatrix} = \begin{pmatrix} \mathbf{j} & \mathbf{A}_{G}\mathbf{j} & \cdots & (\mathbf{A}_{G})^{p-1}\mathbf{j} \end{pmatrix} \underbrace{\begin{pmatrix} \alpha_{11} & \cdots & \alpha_{1p} \\ \vdots & \ddots & \vdots \\ \alpha_{p1} & \cdots & \alpha_{pp} \end{pmatrix}}_{:=\mathbf{Q}} = \mathbf{W}_{G}\mathbf{Q}.$$

The matrix **Q** must be invertible, since $\operatorname{rank}(\mathbf{W}_H) = \operatorname{rank}(\mathbf{W}_G) = p$.

Conversely, in $\mathbf{W}_H = \mathbf{W}_G \mathbf{Q}$ the column vectors of \mathbf{W}_G are combined linearly by the columns of \mathbf{Q} ; so they are vectors in $\operatorname{Main}(G)$. Since \mathbf{Q} is invertible, the linearly independent columns of \mathbf{W}_G span the column space of all of \mathbf{W}_H . Hence they form a basis for both $\operatorname{Main}(H)$ and $\operatorname{Main}(G)$.

Example 15. An example of a pair of graphs G and H having related walk matrices is given in Figure 8. These correspond, respectively, to graphs 31 and 37 from [2], and were pointed out by Curmi [1].

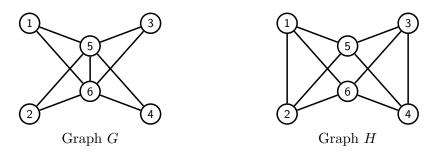


Figure 8. Graphs G and H have the same main eigenspace and related walk matrices.

Indeed we have

$$\mathbf{W}_{G} = \begin{pmatrix} 1 & 2\\ 1 & 2\\ 1 & 2\\ 1 & 2\\ 1 & 5\\ 1 & 5 \end{pmatrix} = \begin{pmatrix} 1 & 3\\ 1 & 3\\ 1 & 3\\ 1 & 3\\ 1 & 4\\ 1 & 4 \end{pmatrix} \begin{pmatrix} 1 & -7\\ 0 & 3 \end{pmatrix} = \mathbf{W}_{H} \begin{pmatrix} 1 & -7\\ 0 & 3 \end{pmatrix} = \mathbf{W}_{H} \mathbf{Q}.$$

This same pair of graphs also serves as a counterexample to the following: graphs that have the same main eigenspace do not necessarily have the same principal main eigenvectors. Indeed, the principal main eigenvectors of G are $(1, 1, 1, 1, \frac{1}{4}(1 \pm \sqrt{33}), \frac{1}{4}(1 \pm \sqrt{33}))$, whereas those of H are $(1, 1, 1, 1, \frac{1}{4}(-1 \pm \sqrt{33}), \frac{1}{4}(-1 \pm \sqrt{33}))$.

The graphs in Figure 3 also have related walk matrices: $\mathbf{W}_G = \begin{pmatrix} 1 & 0 \\ 0 & 2/3 \end{pmatrix} \mathbf{W}_H$.

We end with a section based on the observations of the graphs in Appendix, to be presented below.

Question 16. Let G and H be two graphs with $CDC(G) \simeq CDC(H)$. Do G and H have the same main eigenvalues? This problem is still open.

Remark 17. On at most 8 vertices, all TF-isomorphic graphs are comain. Even though in Appendix, the algorithm narrows the search space to consider graphs on at most 8 vertices, the list is still exhaustive, because it was determined computationally that there are no counterexamples to the conjecture implied by Question 16 on at most 8 vertices.

6. Appendix. All Pairs of TF-isomorphic Graphs on at most 8 Vertices

Here, we give a complete list of all the TF-isomorphic graphs on 8 vertices, that is, all pairs of graphs G, H with $\text{CDC}(G) \simeq \text{CDC}(H)$. Since for any pair of TF-isomorphic graphs, we have

$$CDC(G\dot{\cup}K_1) \simeq CDC(H\dot{\cup}K_1)$$

by Lemma 11, this list contains all possible TF-isomorphic graphs on at most 8 vertices (those pairs with n < 8 vertices will correspond to graphs with isolated vertices added to both, such as the first pair in the table).

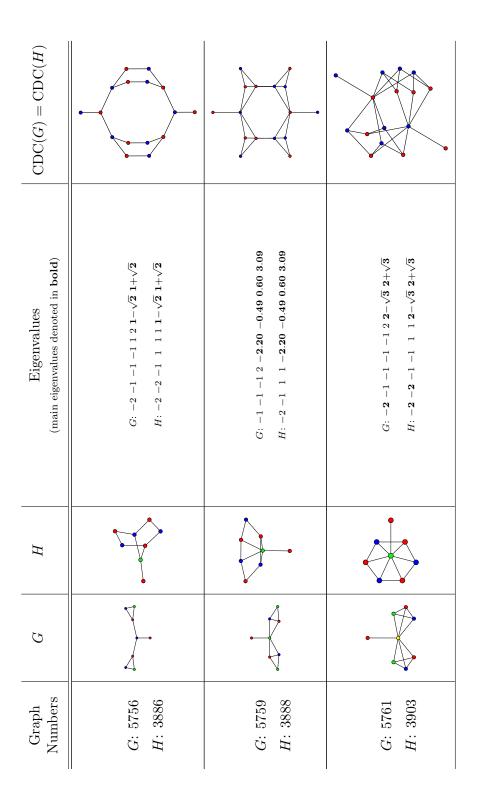
This list was constructed by running a C program which filtered the list of non-isomorphic graphs on 8 vertices available on Brendan McKay's website [8]. First, the large search space of $\binom{12\,346}{2} = 76\,205\,685$ pairs of non-isomorphic graphs was significantly reduced to 1595 pairs of graphs which are comain using the QR algorithm, a step that is justified by Remark 17. This was the most intensive step computationally. Then another program found the CDC of each of the remaining graphs, and these were compared pairwise to check for isomorphism.

The "graph numbers" below correspond to the numbering given in McKay's list for non-isomorphic graphs on 8 CDC(G) = CDC(H)• $G: -1 \ 1 \ -1.48 \ 0.31 \ 2.17 \ -2.17 \ -0.31 \ 1.48$ $H: -1 -1 -1.48 -1.48 \ 0.31 \ 0.31 \ 2.17 \ 2.17$ (main eigenvalues denoted in **bold**) G: -2 -1 0 1 1 -1.81 0.47 2.34 $H: -1 -1 -1 \ 0 \ 2 \ -1.81 \ 0.47 \ 2.34$ G: -1 -1 -1 -1 0 0 2 2 $H: -2 -1 -1 \ 0 \ 0 \ 1 \ 1 \ 2$ Eigenvalues Η • \mathcal{O} Numbers G: 958G: 1162G: 1164H: 1032Graph H: 447H: 1030vertices¹.

¹The images of the graphs were generated by importing the output of the C program into Mathematica. The vertices are coloured using an implementation of Brélaz's colouring algorithm. This produces a near-optimal vertex colouring for all the graphs.

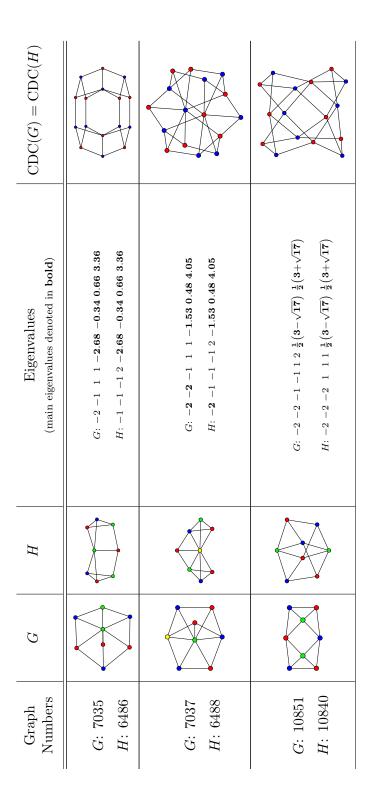
CDC(G) = CDC(H)				
Eigenvalues (main eigenvalues denoted in bold)	$G: -2 -1 \ 0 \ 1 \ 1 -2.32 \ 0.64 \ 2.68$ $H: -1 -1 \ 0 \ 2 -2.32 \ 0.64 \ 2.68$	$G: -1 -1 \ 0 \ 0 \ \frac{1}{2} \left(1 - \sqrt{17}\right) \ \frac{1}{2} \left(1 - \sqrt{17}\right) \ \frac{1}{2} \left(1 - \sqrt{17}\right) \ \frac{1}{2} \left(1 + \sqrt{17}\right) \ \frac{1}{2} \left(1 + \sqrt{17}\right) $ $H: -1 \ 0 \ 0 \ 1 \ \frac{1}{2} \left(-1 - \sqrt{17}\right) \ \frac{1}{2} \left(1 - \sqrt{17}\right) \ \frac{1}{2} \left(\sqrt{17} - 1\right) \ \frac{1}{2} \left(1 + \sqrt{17}\right) $	G: $-1 -1 -2.27$ 0.14 3.13 -1.48 0.31 2.17 H: $-1 1 -2.27$ 0.14 3.13 $-2.17 -0.31$ 1.48	$G: -2 -2 \ 0 \ 1 \ 1 \ 1 \ \frac{1}{2} \left(1 - \sqrt{17} \right) \ \frac{1}{2} \left(1 + \sqrt{17} \right)$ $H: -2 -1 \ -1 \ 0 \ 1 \ 2 \ \frac{1}{2} \left(1 - \sqrt{17} \right) \ \frac{1}{2} \left(1 + \sqrt{17} \right)$
Н	X			\bigwedge
U		$\overleftrightarrow \overleftrightarrow$	A A	
Graph Numbers	G: 1235 H: 1105	G: 3494 H: 3392	$G: 3592 \ H: 3482$	G: 3779 H: 3413

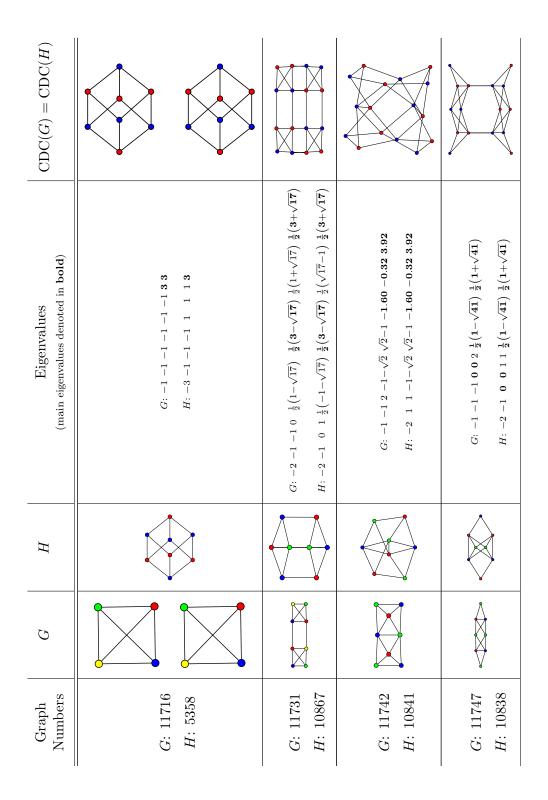
CDC(G) = CDC(H)				•
Eigenvalues (main eigenvalues denoted in bold)	G: $-1 - 1 - 1 - 1$ 1 2 2 H: $-2 - 1 - 1 - 1$ 1 1 1 2	G: -2 -2 -1 -1 1 1 1 3 H: -2 -1 -1 -1 -1 2 3	G: $-2 -1 -1 -1 0 0 2 3H$: $-2 -2 -1 0 0 1 1 3$	$G: -1 -1 -1 -1 0 2 1 - \sqrt{7} 1 + \sqrt{7}$ $H: -2 -1 -1 0 1 1 1 - \sqrt{7} 1 + \sqrt{7}$
Н		X	È.	
G				\$.
Graph Numbers	$G: 5629 \ H: 1270$	G: 5718 H: 5684	G: 5753 H: 3887	G: 5755 H: 3899



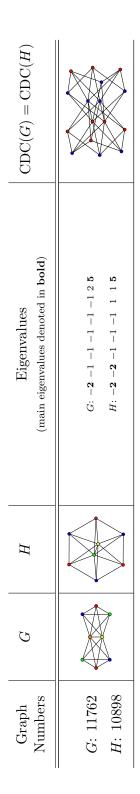
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CDC(G) = CDC(H)						
Eigenvalues (main eigenvalues denoted in bold)	G: -2 0 1 1 -2.29 -1.48 0.55 3.21 H: -1 -1 0 2 -2.29 -1.48 0.55 3.21	G : -2 1 1 -1- $\sqrt{2}$ $\sqrt{2}$ -1 -1.34 0.53 2.81 H : -1 -1 2 -1- $\sqrt{2}$ $\sqrt{2}$ -1 -1.34 0.53 2.81	$G: -2 -2 \ 1 \ 1 -1.79 \ -0.28 \ 0.56 \ 3.52$ $H: -2 -1 -1 \ 2 -1.79 \ -0.28 \ 0.56 \ 3.52$	G: -2 -1 -1 1 1 -2.25 1.15 3.10 H: -1 -1 -1 -1 2 -2.25 1.15 3.10	G: -2 -2 -1 1 1 -1.49 0.71 3.78 H: -2 -1 -1 2 -1.49 0.71 3.78	
Н	\mathbf{A}	$\bigcup_{i=1}^{k}$			$\overset{}{\checkmark}$	
IJ		X				
Graph Numbers	G: 7012 H: 6471	G: 7013 H: 6479	G: 7015 H: 6481	G: 7026 H: 6476	G: 7028 H: 6478	





CDC(G) = CDC(H)					
Eigenvalues (main eigenvalues denoted in bold)	G: $-1 - 1 - 1 - 1 2 - 2.30 0.21 4.08H$: $-2 - 1 - 1 1 - 2.30 0.21 4.08$	G: $-1 -1 -1 2 -2.39 -1.35 0.60 4.14H$: $-2 -1 1 1 -2.39 -1.35 0.60 4.14$	G: -2 -1 -1 -1 2 -1.64 0.14 4.50 H: -2 -2 -1 1 1 -1.64 0.14 4.50	G: $-1 -1 -2.38 -0.72 4.10 -1.48 0.31 2.17H$: $-1 1 -2.38 -0.72 4.10 -2.17 -0.31 1.48$	$G: -1 -1 -1 -1 0 2 1 - \sqrt{13} 1 + \sqrt{13}$ $H: -2 -1 -1 0 1 1 1 - \sqrt{13} 1 + \sqrt{13}$
Н					
U	Ř			A	
Graph Numbers	G: 11748 H: 10839	G: 11751 H: 10849	G: 11752 H: 10850	G: 11755 H: 10887	G: 11761 H: 10897



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