

On pseudo walk matrices

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Abstract

A pseudo walk matrix associated with a graph G having adjacency matrix \mathbf{A} is a matrix with columns $\mathbf{v}, \mathbf{A}\mathbf{v}, \mathbf{A}^2\mathbf{v}, \dots, \mathbf{A}^{r-1}\mathbf{v}$ (for a specific r) where the Gram matrix of these columns contains particular walk enumerations in G . For any subset S of the Cartesian product of the vertex set $\mathcal{V}(G)$ with itself, we consider the total number of walks $N_0(S), N_1(S), N_2(S), \dots$ of length $0, 1, 2, \dots$ in G that start from vertex i and end at vertex j for all $(i, j) \in S$. We present a method that, given such a set S , produces a walk vector \mathbf{v} (with possibly complex entries) such that the Gram matrix of the columns of the pseudo walk matrix resulting from this walk vector is the Hankel matrix whose skew diagonals contain the values $N_0(S), \dots, N_{2r-2}(S)$. Various results on such pseudo walk matrices are derived, particularly on closed pseudo walk matrices whose set S contains only the pairs (v, v) for all $v \in \mathcal{V}(G)$. Moreover, a result akin to the classic Harary-Sachs coefficient theorem in chemical graph theory that computes any coefficient of the characteristic polynomial of the companion matrix of a pseudo walk matrix is conveyed.

Keywords: graph walks; pseudo walk matrix; walk vector; coefficient theorem; closed pseudo walk matrix.

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1. Introduction

Let G be a simple graph on n vertices, having vertex set $\mathcal{V}(G)$ and adjacency matrix \mathbf{A} . The eigenvalues and eigenvectors of G are those of \mathbf{A} , where each eigenvalue λ of G satisfies $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ for some nonzero eigenvector \mathbf{x} in the eigenspace of λ . Since \mathbf{A} is a real and symmetric matrix, there exists an orthonormal set of n eigenvectors $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ of \mathbf{A} . Thus $\mathbf{A} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^T$, where \mathbf{X} is an orthogonal matrix whose columns are $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, \mathbf{X}^T is its transpose, and $\mathbf{\Lambda}$ is the diagonal matrix whose main diagonal entries are the (possibly not distinct) eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$.

We denote the entry in the i^{th} row and j^{th} column of any matrix \mathbf{M} by $[\mathbf{M}]_{ij}$; similarly, we denote the k^{th} entry of a vector \mathbf{v} by $[\mathbf{v}]_k$. We remark that $[\mathbf{M}]_{ij} = \mathbf{e}_i^T \mathbf{M} \mathbf{e}_j$, where \mathbf{e}_k is the k^{th} column of the identity matrix \mathbf{I} ; analogously, $[\mathbf{v}]_k = \mathbf{e}_k^T \mathbf{v}$. If \mathbf{M} is a square matrix, then $|\mathbf{M}|$ denotes its determinant. A Hankel matrix is a square matrix with constant skew diagonal entries. The entries of the vector \mathbf{j} are all equal to 1.

A walk of length ℓ in G , starting from $u \in \mathcal{V}(G)$ and ending at $v \in \mathcal{V}(G)$, is a sequence of ℓ edges e_1, e_2, \dots, e_ℓ such that e_1 is incident to u , e_ℓ is incident to v and the two edges e_j, e_{j+1} share a vertex for all $j = 1, 2, \dots, \ell - 1$. Note that neither these edges nor the vertices u and v need to be distinct. If $u = v$, then the walk is closed.

Let S be any subset of the set $\mathcal{V}^2 = \mathcal{V}(G) \times \mathcal{V}(G)$. For any non-negative integer k , we focus our attention on the walks of length k in G that start from vertex u and end at vertex v for all pairs (u, v) in S . We denote the total number of all such walks by $N_k(S)$. It is well-known [1, 3] that

$$N_k(S) = \sum_{(u,v) \in S} [\mathbf{A}^k]_{uv}. \quad (1)$$

In the literature, the *walk matrix* \mathbf{W} associated with a graph G is either the $n \times n$ matrix $(\mathbf{j} \quad \mathbf{A}\mathbf{j} \quad \mathbf{A}^2\mathbf{j} \quad \dots \quad \mathbf{A}^{n-1}\mathbf{j})$ [4, 7, 8] or the $n \times r$ matrix $(\mathbf{j} \quad \mathbf{A}\mathbf{j} \quad \mathbf{A}^2\mathbf{j} \quad \dots \quad \mathbf{A}^{r-1}\mathbf{j})$ where r is the smallest value for this matrix to attain its maximum column rank [2, 12]. Here, we shall adopt the second definition of a walk matrix, that is, the one having r columns. Note that the matrix $(\mathbf{j} \quad \mathbf{A}\mathbf{j} \quad \mathbf{A}^2\mathbf{j} \quad \dots \quad \mathbf{A}^{p-1}\mathbf{j})$ has rank r for all $p \geq r$ and has rank p for all $1 \leq p \leq r$ [12, 13]. It is known that r is the number of *main eigenvalues* of G , that is, the number of eigenvalues of G having an eigenvector in their eigenspace whose entries sum up to a nonzero number [9]. Moreover, G is a regular graph if and only if $r = 1$ [13], while G is a controllable graph if and only if $r = n$ [4, 8]. By (1), the entry $[\mathbf{W}]_{ij}$ is equal to $N_{j-1}(S_i)$, where $S_i = \{(i, k) \mid k \in \mathcal{V}(G)\}$.

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The matrix $\mathbf{W}^\top \mathbf{W}$, that is, the Gram matrix of the columns of \mathbf{W} , is a positive semidefinite Hankel matrix where $[\mathbf{W}^\top \mathbf{W}]_{ij}$ is equal to $N_{i+j-2}(\mathcal{V}^2)$ for all i, j . Note that the previous sentence is true irrespective of the number of columns of \mathbf{W} . It is well-known that \mathbf{W} and $\mathbf{W}^\top \mathbf{W}$ have the same rank [11]; thus, $\mathbf{W}^\top \mathbf{W}$ is an $r \times r$ invertible (and, hence, positive definite) matrix. In this sense, we can say that the vector \mathbf{j} is a *walk vector* for \mathcal{V}^2 , because an $n \times r$ walk matrix \mathbf{W} having the r linearly independent columns $\mathbf{j}, \mathbf{A}\mathbf{j}, \dots, \mathbf{A}^{r-1}\mathbf{j}$ produces a Hankel matrix $\mathbf{W}^\top \mathbf{W}$ containing the walk enumerations $N_0(\mathcal{V}^2), N_1(\mathcal{V}^2), \dots, N_{2r-2}(\mathcal{V}^2)$ on its $(2r-1)$ skew diagonals.

The purpose of this paper is to obtain walk vectors for any $S \subseteq \mathcal{V}^2$. In other words, given a subset S of \mathcal{V}^2 , we produce a vector \mathbf{v} such that the Gram matrix of the columns of $\mathbf{W}_{\mathbf{v}} = (\mathbf{v} \ \mathbf{A}\mathbf{v} \ \mathbf{A}^2\mathbf{v} \ \dots \ \mathbf{A}^{r-1}\mathbf{v})$, where r is the least value that maximizes the rank of $\mathbf{W}_{\mathbf{v}}$, is a Hankel matrix containing the walk enumerations $N_0(S), N_1(S), \dots, N_{2r-2}(S)$ on its skew diagonals. We shall show, in Theorem 3.1, that this is possible for any S ; indeed, different suitable walk vectors associated with a given set S usually exist. Unfortunately, often \mathbf{v} does not end up being a 0–1 vector, in which case, the matrix $\mathbf{W}_{\mathbf{v}}$ itself would not contain walk enumerations, even though $\mathbf{W}_{\mathbf{v}}^\top \mathbf{W}_{\mathbf{v}}$ would. If this is the case, then we call $\mathbf{W}_{\mathbf{v}}$ a *pseudo walk matrix* associated with S .

The following definition summarizes the terminology introduced thus far.

Definition 1.1. A **pseudo walk matrix** $\mathbf{W}_{\mathbf{v}}$ associated with $S \subseteq \mathcal{V}^2$ is a matrix of the form $(\mathbf{v} \ \mathbf{A}\mathbf{v} \ \mathbf{A}^2\mathbf{v} \ \dots \ \mathbf{A}^{r-1}\mathbf{v})$ such that r is the smallest value for which the rank of $\mathbf{W}_{\mathbf{v}}$ is maximum and, for all i and j ,

$$[\mathbf{W}_{\mathbf{v}}^\top \mathbf{W}_{\mathbf{v}}]_{ij} = N_{i+j-2}(S).$$

The vector \mathbf{v} in the previous sentence is a **walk vector** associated with S . If \mathbf{v} is a 0–1 vector, then $\mathbf{W}_{\mathbf{v}}$ may be simply called a **walk matrix** associated with S .

Thus, the walk matrix associated with the entire set \mathcal{V}^2 , which is the walk matrix usually alluded to in the literature, is represented in this work by $\mathbf{W}_{\mathbf{j}}$.

2. Useful results

Before proving our main result in Theorem 3.1 that pseudo walk matrices exist for any set $S \subseteq \mathcal{V}^2$, we first present some results on pseudo walk matrices that are analogous to those for walk matrices found in the literature.

We mentioned earlier that the rank of the walk matrix $\mathbf{W}_{\mathbf{j}}$ (and hence, its number of columns) is equal to the number of main eigenvalues of G [9]. We have an analogous result for pseudo walk matrices $\mathbf{W}_{\mathbf{v}}$ in Theorem 2.1 below. This result also tells us that if we manage to obtain a suitable pseudo walk matrix $\mathbf{W}_{\mathbf{v}}$ for the set $S \subseteq \mathcal{V}^2$, then it has the same rank as any other suitable one that uses a walk vector different from \mathbf{v} .

Theorem 2.1. The number of columns r of any pseudo walk matrix $\mathbf{W}_{\mathbf{v}} = (\mathbf{v} \ \mathbf{A}\mathbf{v} \ \mathbf{A}^2\mathbf{v} \ \dots \ \mathbf{A}^{r-1}\mathbf{v})$ associated with $S \subseteq \mathcal{V}^2$ (so that any further columns $\mathbf{A}^r\mathbf{v}, \mathbf{A}^{r+1}\mathbf{v}, \dots$ would not increase its rank) is equal to the number of eigenvalues of G having an eigenvector not orthogonal to \mathbf{v} . Moreover, if \mathbf{v}_1 and \mathbf{v}_2 are two distinct walk vectors associated with S , then $\mathbf{W}_{\mathbf{v}_1}$ and $\mathbf{W}_{\mathbf{v}_2}$ have the same rank.

Proof. We assume that if a particular eigenvalue λ of G is repeated t times, then we choose its eigenvectors $\mathbf{x}_i, \dots, \mathbf{x}_{i+t-1}$ so that at least $(t-1)$ of them are orthogonal to \mathbf{v} . (If \mathbf{x}_i and \mathbf{x}_{i+1} are both not orthogonal to \mathbf{v} , then replace one of them by $(\mathbf{v}^\top \mathbf{x}_i)\mathbf{x}_{i+1} - (\mathbf{v}^\top \mathbf{x}_{i+1})\mathbf{x}_i$, and repeat until at least $(t-1)$ of $\mathbf{x}_i, \dots, \mathbf{x}_{i+t-1}$ are orthogonal to \mathbf{v} .) Since the columns of \mathbf{X} span \mathbb{R}^n , we may express \mathbf{v} as $\sum_{j=1}^n v_j \mathbf{x}_j$ for constants v_1, \dots, v_n ; moreover, $v_j = \mathbf{v}^\top \mathbf{x}_j$ for all j , since the columns of \mathbf{X} are mutually orthogonal. This means that $\mathbf{A}^k \mathbf{v} = \sum_{j=1}^n (\mathbf{v}^\top \mathbf{x}_j) \lambda_j^k \mathbf{x}_j$ for any non-negative integer k . Hence

$$\mathbf{A}^k \mathbf{v} = (\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_n) \begin{pmatrix} (\mathbf{v}^\top \mathbf{x}_1) \lambda_1^k & (\mathbf{v}^\top \mathbf{x}_2) \lambda_2^k & \dots & (\mathbf{v}^\top \mathbf{x}_n) \lambda_n^k \end{pmatrix}^\top.$$

Consider the $n \times n$ matrix $\mathbf{W}'_{\mathbf{v}} = (\mathbf{v} \ \mathbf{A}\mathbf{v} \ \mathbf{A}^2\mathbf{v} \ \dots \ \mathbf{A}^{n-1}\mathbf{v})$, which has the same rank as the pseudo walk matrix $\mathbf{W}_{\mathbf{v}}$. We have:

$$\mathbf{W}'_{\mathbf{v}} = (\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_n) \begin{pmatrix} (\mathbf{v}^\top \mathbf{x}_1) & (\mathbf{v}^\top \mathbf{x}_1) \lambda_1 & \dots & (\mathbf{v}^\top \mathbf{x}_1) \lambda_1^{n-1} \\ (\mathbf{v}^\top \mathbf{x}_2) & (\mathbf{v}^\top \mathbf{x}_2) \lambda_2 & \dots & (\mathbf{v}^\top \mathbf{x}_2) \lambda_2^{n-1} \\ \vdots & \vdots & & \vdots \\ (\mathbf{v}^\top \mathbf{x}_n) & (\mathbf{v}^\top \mathbf{x}_n) \lambda_n & \dots & (\mathbf{v}^\top \mathbf{x}_n) \lambda_n^{n-1} \end{pmatrix}. \quad (2)$$

Since $(\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_n)$ has full rank, the rank of $\mathbf{W}'_{\mathbf{v}}$ is equal to the rank of the matrix

$$\mathbf{M} = \begin{pmatrix} (\mathbf{v}^\top \mathbf{x}_1) & (\mathbf{v}^\top \mathbf{x}_1) \lambda_1 & \dots & (\mathbf{v}^\top \mathbf{x}_1) \lambda_1^{n-1} \\ (\mathbf{v}^\top \mathbf{x}_2) & (\mathbf{v}^\top \mathbf{x}_2) \lambda_2 & \dots & (\mathbf{v}^\top \mathbf{x}_2) \lambda_2^{n-1} \\ \vdots & \vdots & & \vdots \\ (\mathbf{v}^\top \mathbf{x}_n) & (\mathbf{v}^\top \mathbf{x}_n) \lambda_n & \dots & (\mathbf{v}^\top \mathbf{x}_n) \lambda_n^{n-1} \end{pmatrix}.$$

Let r be the number of eigenvalues of G that have an eigenvector not orthogonal to \mathbf{v} . Then \mathbf{M} has exactly r nonzero rows, and consequently, the rank of \mathbf{M} is at most equal to r . We now show that the rank of \mathbf{M} is exactly r . Let \mathbf{M}' be the $r \times r$ submatrix obtained from \mathbf{M} by removing its zero rows and its last $(n - r)$ columns, so that

$$\mathbf{M}' = \begin{pmatrix} (\mathbf{v}^\top \mathbf{y}_1) & (\mathbf{v}^\top \mathbf{y}_1)\mu_1 & \cdots & (\mathbf{v}^\top \mathbf{y}_1)\mu_1^{r-1} \\ (\mathbf{v}^\top \mathbf{y}_2) & (\mathbf{v}^\top \mathbf{y}_2)\mu_2 & \cdots & (\mathbf{v}^\top \mathbf{y}_2)\mu_2^{r-1} \\ \vdots & \vdots & & \vdots \\ (\mathbf{v}^\top \mathbf{y}_r) & (\mathbf{v}^\top \mathbf{y}_r)\mu_r & \cdots & (\mathbf{v}^\top \mathbf{y}_r)\mu_r^{r-1} \end{pmatrix}$$

where $\mathbf{y}_1, \dots, \mathbf{y}_r$ are the r eigenvectors of \mathbf{A} that are not orthogonal to \mathbf{v} and that are associated with the eigenvalues μ_1, \dots, μ_r respectively. Note that μ_1, \dots, μ_r are distinct, since we have ensured that only one eigenvector in the eigenbasis of μ_i is not orthogonal to \mathbf{v} . The determinant of \mathbf{M}' is

$$\left(\prod_{i=1}^r (\mathbf{v}^\top \mathbf{y}_i) \right) \begin{vmatrix} 1 & \mu_1 & \cdots & \mu_1^{r-1} \\ 1 & \mu_2 & \cdots & \mu_2^{r-1} \\ \vdots & \vdots & & \vdots \\ 1 & \mu_r & \cdots & \mu_r^{r-1} \end{vmatrix}.$$

But the above determinant is that of a Vandermonde matrix, which is known to be nonzero if and only if the eigenvalues μ_1, \dots, μ_r are distinct [11, p. 37]. Since $\mathbf{v}^\top \mathbf{y}_i \neq 0$ for all $i \in \{1, 2, \dots, r\}$ as well, $|\mathbf{M}'|$ is nonzero. Consequently, the order of the largest non-vanishing minor of \mathbf{M} is r , which means that the (determinantal) rank of $\mathbf{W}'_{\mathbf{v}}$ is r . Thus, $\mathbf{W}_{\mathbf{v}}$ must have r columns.

Finally, suppose $\mathbf{W}_{\mathbf{v}_1}$ and $\mathbf{W}_{\mathbf{v}_2}$ are both pseudo walk matrices for the set S , and the former has r_1 columns while the latter has r_2 columns, where $r_1 \leq r_2$. Recall that r_1 is the smallest number of columns such that $\mathbf{W}_{\mathbf{v}_1}$ has maximum rank; an analogous statement can be said for r_2 and $\mathbf{W}_{\mathbf{v}_2}$. Then $\mathbf{H}_1 = \mathbf{W}_{\mathbf{v}_1}^\top \mathbf{W}_{\mathbf{v}_1}$ has rank r_1 and $\mathbf{H}_2 = \mathbf{W}_{\mathbf{v}_2}^\top \mathbf{W}_{\mathbf{v}_2}$ has rank r_2 . But the upper left $r_1 \times r_1$ submatrix of \mathbf{H}_2 is \mathbf{H}_1 , since $\mathbf{W}_{\mathbf{v}_1}$ and $\mathbf{W}_{\mathbf{v}_2}$ are both pseudo walk matrices associated with S . Moreover, \mathbf{H}_1 and \mathbf{H}_2 are both invertible. This means that $\mathbf{W}_{\mathbf{v}_1}$ must have r_2 columns, so $r_1 = r_2$, as required. \square

The following two corollaries are immediate.

Corollary 2.1. *For any $S \subseteq \mathcal{V}^2$, the number of distinct eigenvalues of G is an upper bound for the number of columns of any pseudo walk matrix associated with S .*

Proof. By Theorem 2.1, the number of columns of $\mathbf{W}_{\mathbf{v}}$ is the number of eigenvalues of G having an eigenvector not orthogonal to \mathbf{v} . This number is the maximum possible whenever each and every distinct eigenvalue of G has such an eigenvector in its eigenspace. \square

We conclude, from Corollary 2.1, that if any pseudo walk matrix has rank n , then G has n distinct eigenvalues. Moreover, we shall show in Theorem 4.2 that the upper bound mentioned in Corollary 2.1 is always attained by a particular pseudo walk matrix for all graphs G .

Powers and Sulaiman in [12] describe the *companion matrix* $\mathbf{C}_{\mathbf{j}}$ as being the $r \times r$ matrix satisfying $\mathbf{A}\mathbf{W}_{\mathbf{j}} = \mathbf{W}_{\mathbf{j}}\mathbf{C}_{\mathbf{j}}$. It is clear that the first $(r - 1)$ columns of $\mathbf{C}_{\mathbf{j}}$ must be $\mathbf{e}_2, \dots, \mathbf{e}_r$. On the other hand, the last column \mathbf{c} satisfies $\mathbf{A}^r \mathbf{j} = \mathbf{W}_{\mathbf{j}}\mathbf{c}$, from which we obtain $\mathbf{c} = (\mathbf{W}_{\mathbf{j}}^\top \mathbf{W}_{\mathbf{j}})^{-1} \mathbf{A}^r \mathbf{j}$ [5]. Note also that the characteristic polynomial of $\mathbf{C}_{\mathbf{j}}$ is $x^r - c_{r-1}x^{r-1} - c_{r-2}x^{r-2} - \cdots - c_0$, where $(c_0 \ c_1 \ \cdots \ c_{r-1})^\top = \mathbf{c}$ — this can be derived simply by employing the usual Laplace determinant expansion along the last column of $x\mathbf{I} - \mathbf{C}_{\mathbf{j}}$. A much more important result is that this characteristic polynomial is $\prod (x - \lambda_k)$, where the product runs over the main eigenvalues λ_k of G [12, Theorem 4].

All of these results carry over for pseudo walk matrices in a natural way, by replacing the vector \mathbf{j} with \mathbf{v} in their respective proofs.

Theorem 2.2. *The companion matrix $\mathbf{C}_{\mathbf{v}}$ of the pseudo walk matrix $\mathbf{W}_{\mathbf{v}}$ satisfying $\mathbf{A}\mathbf{W}_{\mathbf{v}} = \mathbf{W}_{\mathbf{v}}\mathbf{C}_{\mathbf{v}}$ is the $r \times r$ matrix $(\mathbf{e}_2 \ \mathbf{e}_3 \ \cdots \ \mathbf{e}_r \ \mathbf{c}_{\mathbf{v}})$, where the column $\mathbf{c}_{\mathbf{v}} = (c_0 \ c_1 \ \cdots \ c_{r-1})^\top = (\mathbf{W}_{\mathbf{v}}^\top \mathbf{W}_{\mathbf{v}})^{-1} \mathbf{A}^r \mathbf{v}$. Moreover, the characteristic polynomial of $\mathbf{C}_{\mathbf{v}}$ is $x^r - c_{r-1}x^{r-1} - c_{r-2}x^{r-2} - \cdots - c_0$, which is equal to the product $\prod (x - \lambda_k)$ running over the eigenvalues λ_k of G that have an eigenvector not orthogonal to \mathbf{v} .*

An immediate corollary of Theorem 2.2 is the following.

Corollary 2.2. *The characteristic polynomial of the companion matrix of any pseudo walk matrix divides the minimal polynomial of G .*

In this paper, we contribute a Cramer-like rule to produce the coefficients of the characteristic polynomial of \mathbf{C}_v from the $2r$ walk enumerations $N_0(S), N_1(S), \dots, N_{2r-1}(S)$.

Theorem 2.3. *The coefficient of x^k of the characteristic polynomial of \mathbf{C}_v is $(-1)^{r-k} \frac{|\mathbf{N}|}{|\mathbf{H}|}$, where $\mathbf{H} = \mathbf{W}_v^\top \mathbf{W}_v$ and \mathbf{N} is the matrix whose first k columns are those of \mathbf{H} and whose last $r - k$ columns are those of $\mathbf{H}' = \mathbf{W}_v^\top \mathbf{A} \mathbf{W}_v$.*

Proof. We start from the relation $\mathbf{W}_v^\top (x\mathbf{I} - \mathbf{A}) \mathbf{W}_v = \mathbf{W}_v^\top \mathbf{W}_v (x\mathbf{I} - \mathbf{C}_v)$, from which we get

$$|x\mathbf{I} - \mathbf{C}_v| = \frac{1}{|\mathbf{H}|} |x\mathbf{H} - \mathbf{H}'|.$$

We note that \mathbf{H} is the Hankel matrix whose columns are $\mathbf{w}_0, \mathbf{w}_1, \dots, \mathbf{w}_{r-1}$, where

$$\mathbf{w}_i = (N_i(S) \quad N_{i+1}(S) \quad \cdots \quad N_{i+r-1}(S))^\top$$

for all i . Moreover, the columns of the Hankel matrix \mathbf{H}' are $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_r$. Thus

$$x\mathbf{H} - \mathbf{H}' = (x\mathbf{w}_0 - \mathbf{w}_1 \quad x\mathbf{w}_1 - \mathbf{w}_2 \quad \cdots \quad x\mathbf{w}_{r-1} - \mathbf{w}_r).$$

By the multilinearity property of the determinant,

$$|x\mathbf{H} - \mathbf{H}'| = x |\mathbf{w}_0 \quad x\mathbf{w}_1 - \mathbf{w}_2 \quad \cdots \quad x\mathbf{w}_{r-1} - \mathbf{w}_r| - |\mathbf{w}_1 \quad x\mathbf{w}_1 - \mathbf{w}_2 \quad \cdots \quad x\mathbf{w}_{r-1} - \mathbf{w}_r|. \quad (3)$$

The second determinant of (3) becomes

$$|\mathbf{w}_1 \quad \mathbf{w}_1 \quad x\mathbf{w}_2 - \mathbf{w}_3 \quad \cdots \quad x\mathbf{w}_{r-1} - \mathbf{w}_r| - |\mathbf{w}_1 \quad \mathbf{w}_2 \quad x\mathbf{w}_2 - \mathbf{w}_3 \quad \cdots \quad x\mathbf{w}_{r-1} - \mathbf{w}_r| \quad (4)$$

so the first determinant in (4) vanishes. By expanding it further in this fashion, the second determinant of (3) is equal to $(-1)^r |\mathbf{w}_1 \quad \mathbf{w}_2 \quad \cdots \quad \mathbf{w}_r|$.

In a similar way, the first determinant of (3) expands to

$$x^r |\mathbf{w}_0 \quad \mathbf{w}_1 \quad \cdots \quad \mathbf{w}_{r-1}| - x^{r-1} |\mathbf{w}_0 \quad \mathbf{w}_1 \quad \cdots \quad \mathbf{w}_{r-2} \quad \mathbf{w}_r| + x^{r-2} |\mathbf{w}_0 \quad \mathbf{w}_1 \quad \cdots \quad \mathbf{w}_{r-3} \quad \mathbf{w}_{r-1} \quad \mathbf{w}_r| - \cdots + (-1)^{r-1} x |\mathbf{w}_0 \quad \mathbf{w}_2 \quad \mathbf{w}_3 \quad \cdots \quad \mathbf{w}_r|.$$

This proves the result. \square

We note that if $v = j$, then Theorem 2.3 above yields the coefficients of the *main characteristic polynomial* [2], that is, the polynomial $\prod_{k=1}^p (x - \mu_k)$ where μ_1, \dots, μ_p are the p main eigenvalues of G (this polynomial is denoted by $m_G(x)$ in [13]). Furthermore, the result in Theorem 2.3 is similar in nature to the classical Harary-Sachs coefficient theorem [10, 14] that determines each coefficient of the characteristic polynomial of any graph from its so-called elementary and basic figures. In Theorem 2.3, we are obtaining each coefficient of the characteristic polynomial of \mathbf{C}_v from the $2r$ walk enumerations $N_0(S), N_1(S), \dots, N_{2r-1}(S)$.

3. Main result

We now come to the main result of this paper, in which, given $S \subseteq \mathcal{V}^2$, a walk vector \mathbf{v} and, consequently, a suitable pseudo walk matrix \mathbf{W}_v , are produced such that the Gram matrix of the columns of \mathbf{W}_v has the walk enumerations $N_0(S), N_1(S), \dots, N_{2r-2}(S)$ on its skew diagonals.

As we did in the proof of Theorem 2.1, we may express \mathbf{e}_u and \mathbf{e}_v as $\sum_{j=1}^n (\mathbf{e}_u^\top \mathbf{x}_j) \mathbf{x}_j$ and $\sum_{j=1}^n (\mathbf{e}_v^\top \mathbf{x}_j) \mathbf{x}_j$ respectively. Hence

$$\begin{aligned} \mathbf{e}_u^\top \mathbf{A}^k \mathbf{e}_v &= \left(\sum_{j=1}^n (\mathbf{e}_u^\top \mathbf{x}_j) \mathbf{x}_j^\top \right) (\mathbf{X} \mathbf{A}^k \mathbf{X}^\top) \left(\sum_{j=1}^n (\mathbf{e}_v^\top \mathbf{x}_j) \mathbf{x}_j \right) \\ &= \left(\sum_{j=1}^n [\mathbf{x}_j]_u (\mathbf{x}_j^\top \mathbf{X}) \right) \mathbf{A}^k \left(\sum_{j=1}^n [\mathbf{x}_j]_v (\mathbf{X}^\top \mathbf{x}_j) \right) \\ &= \left(\sum_{j=1}^n [\mathbf{x}_j]_u \mathbf{e}_j^\top \right) \mathbf{A}^k \left(\sum_{j=1}^n [\mathbf{x}_j]_v \mathbf{e}_j \right) \end{aligned}$$

$$\begin{aligned}
&= \begin{pmatrix} [\mathbf{x}_1]_u & [\mathbf{x}_2]_u & \cdots & [\mathbf{x}_n]_u \end{pmatrix} \begin{pmatrix} \lambda_1^k & 0 & \cdots & 0 \\ 0 & \lambda_2^k & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_n^k \end{pmatrix} \begin{pmatrix} [\mathbf{x}_1]_v \\ [\mathbf{x}_2]_v \\ \vdots \\ [\mathbf{x}_n]_v \end{pmatrix}. \\
&[\mathbf{A}^k]_{uv} = \sum_{j=1}^n [\mathbf{x}_j]_u [\mathbf{x}_j]_v \lambda_j^k.
\end{aligned} \tag{5}$$

Consequently, by combining (1) and (5), and recalling that \mathbf{x}_j is the j^{th} column of \mathbf{X} for all j , the number of walks of length k starting from vertex u and ending at vertex v within all possible pairs (u, v) in S is

$$N_k(S) = \sum_{(u,v) \in S} \left(\sum_{j=1}^n [\mathbf{X}]_{uj} [\mathbf{X}]_{vj} \lambda_j^k \right) = \sum_{j=1}^n \left(\sum_{(u,v) \in S} [\mathbf{X}]_{uj} [\mathbf{X}]_{vj} \right) \lambda_j^k. \tag{6}$$

Now suppose $\mathbf{W}_{\mathbf{v}}$ is a pseudo walk matrix for S with walk vector \mathbf{v} . Then each entry of $\mathbf{W}_{\mathbf{v}}^{\top} \mathbf{W}_{\mathbf{v}}$ is of the form $\mathbf{v}^{\top} \mathbf{A}^k \mathbf{v}$ for some appropriate value of k . Since we may also write down \mathbf{v} as $\sum_{j=1}^n (\mathbf{v}^{\top} \mathbf{x}_j) \mathbf{x}_j$, we may repeat what we did in (5) above, after replacing both \mathbf{e}_u and \mathbf{e}_v with \mathbf{v} , to obtain

$$\mathbf{v}^{\top} \mathbf{A}^k \mathbf{v} = \sum_{j=1}^n (\mathbf{v}^{\top} \mathbf{x}_j)^2 \lambda_j^k. \tag{7}$$

Hence, by comparing (6) and (7), our choice of the walk vector \mathbf{v} will yield the desired results if we force $(\mathbf{v}^{\top} \mathbf{x}_j)^2$ to be equal to $\sum_{(u,v) \in S} [\mathbf{X}]_{uj} [\mathbf{X}]_{vj}$ for all $j = 1, 2, \dots, n$. Thus, let

$$d_j = \pm (\mathbf{v}^{\top} \mathbf{x}_j) = \pm \left(\sum_{(u,v) \in S} [\mathbf{X}]_{uj} [\mathbf{X}]_{vj} \right)^{1/2}, j \in \{1, 2, \dots, n\}$$

where the choice of sign is arbitrary for all j . Note that, for any j , if $d_j \neq 0$, then it is either real or purely imaginary. We now form the vector $\mathbf{d} = (d_1 \ d_2 \ \cdots \ d_n)^{\top}$; we have up to 2^n different options for \mathbf{d} , depending on our choice of sign for each of its entries.

But since $\mathbf{v} = \sum_{j=1}^n (\mathbf{v}^{\top} \mathbf{x}_j) \mathbf{x}_j$, we have

$$\mathbf{X}^{\top} \mathbf{v} = \sum_{j=1}^n (\mathbf{v}^{\top} \mathbf{x}_j) (\mathbf{X}^{\top} \mathbf{x}_j) = \sum_{j=1}^n d_j \mathbf{e}_j = \mathbf{d}.$$

Consequently, $\mathbf{v} = \mathbf{X} \mathbf{d}$, and we obtain the main result of this paper.

Theorem 3.1. *Let S be any subset of \mathcal{V}^2 . Then \mathbf{v} is a walk vector associated with S if $\mathbf{v} = \mathbf{X} \mathbf{d}$, where \mathbf{X} is an orthogonal matrix whose columns are n orthonormal eigenvectors of G associated with its n (possibly not distinct) eigenvalues and \mathbf{d} is any column vector where, for $k = 1, 2, \dots, n$, $[\mathbf{d}]_k = \pm \sqrt{\sum_{(u,v) \in S} [\mathbf{X}]_{uk} [\mathbf{X}]_{vk}}$.*

Thus, by Theorem 3.1, possible walk vectors for S may be found using just \mathbf{X} , an $n \times n$ matrix of orthonormal eigenvectors of G . Moreover, if \mathbf{d} contains at least one purely imaginary entry, then \mathbf{v} may contain complex entries, and hence, so would the pseudo walk matrix $\mathbf{W}_{\mathbf{v}}$ associated with S .

If we have two disjoint subsets S_1 and S_2 of \mathcal{V}^2 , then a simple application of Theorem 3.1 yields the walk vector for $S_1 \cup S_2$ from those of S_1 and S_2 , which is the next corollary.

Corollary 3.1. *Let S_1 and S_2 be two disjoint subsets of \mathcal{V}^2 , having walk vectors \mathbf{v}_1 and \mathbf{v}_2 respectively. Then a suitable walk vector for $S_1 \cup S_2$ is $\mathbf{X} \mathbf{d}$, where, for all i , $[\mathbf{d}]_i$ satisfies*

$$[\mathbf{d}]_i^2 = [\mathbf{X}^{\top} \mathbf{v}_1]_i^2 + [\mathbf{X}^{\top} \mathbf{v}_2]_i^2.$$

Recall that any pseudo walk matrix is a walk matrix if and only if its walk vector is a 0–1 vector. Such a 0–1 walk vector is clearly the walk matrix associated with $V \times V$ where V is some subset of $\mathcal{V}(G)$. Thus, if $S \neq V \times V$ for some $V \subseteq \mathcal{V}(G)$, then every walk vector associated with S produces a pseudo walk matrix that is not a walk matrix.

4. Closed pseudo walk matrices

A *closed pseudo walk matrix* is any pseudo walk matrix associated with the set $C = \{(v, v) \mid v \in \mathcal{V}(G)\}$. The Gram matrix of the columns of any closed pseudo walk matrix contains the number of all *closed* walks of length $0, 1, 2, \dots, 2s-2$ in G . Walk vectors associated with closed pseudo walk matrices have a special form.

Theorem 4.1. *Any one of the 2^n vectors $\pm \mathbf{x}_1 \pm \mathbf{x}_2 \pm \dots \pm \mathbf{x}_n$ is a walk vector for closed pseudo walk matrices associated with C .*

Proof. By Theorem 3.1, the walk vector \mathbf{v} associated with C is $\mathbf{X}\mathbf{d}$, where

$$[\mathbf{d}]_i = \pm \sqrt{[\mathbf{X}]_{i1}^2 + \dots + [\mathbf{X}]_{in}^2}$$

for all i . The result follows since \mathbf{X} is orthogonal, and hence \mathbf{d} ends up being the vector $(\pm 1 \ \pm 1 \ \dots \ \pm 1)^T$. \square

Closed pseudo walk matrices have the maximum number of columns allowed by Theorem 2.1.

Theorem 4.2. *The number of columns of any closed pseudo walk matrix is equal to s , the number of distinct eigenvalues of G .*

Proof. By Theorem 4.1, a suitable walk vector for any closed pseudo walk matrix is $\mathbf{v} = \mathbf{X}\mathbf{j}$. Since $\mathbf{x}_i^T \mathbf{X}\mathbf{j} = \mathbf{e}_i^T \mathbf{j} = 1 \neq 0$ for all i , all eigenvalues of \mathbf{A} have an eigenvector that is not orthogonal to $\mathbf{X}\mathbf{j}$. By Theorem 2.1, any closed pseudo walk matrix must have as many columns as the number of distinct eigenvalues of G . \square

Note that closed pseudo walk matrices may not be the only pseudo walk matrices that have the maximum rank s . Theorem 4.2 is simply assuring us that we have at least one $n \times s$ pseudo walk matrix at our disposal.

Corollary 4.1. *Any pseudo walk matrix has at most as many columns as any closed pseudo walk matrix.*

Proof. Immediate by combining Theorem 2.1 and Theorem 4.2. \square

We also have the following interesting result as a direct consequence of Corollary 2.2 and Theorem 4.2.

Theorem 4.3. *The characteristic polynomial of the companion matrix of any closed pseudo walk matrix is the minimal polynomial of G .*

The coefficients of the minimal polynomial of G may thus be calculated by Theorem 2.3.

Theorem 4.4. *The coefficient of x^k of the minimal polynomial of G , having s distinct eigenvalues, is $(-1)^{r-k} \frac{|\mathbf{N}|}{|\mathbf{H}|}$, where*

$$\mathbf{H} = \begin{pmatrix} N_0(C) & N_1(C) & \cdots & N_{s-1}(C) \\ N_1(C) & N_2(C) & \cdots & N_s(C) \\ \vdots & \vdots & & \vdots \\ N_{s-1}(C) & N_s(C) & \cdots & N_{2s-2}(C) \end{pmatrix}, \quad \mathbf{H}' = \begin{pmatrix} N_1(C) & N_2(C) & \cdots & N_s(C) \\ N_2(C) & N_3(C) & \cdots & N_{s+1}(C) \\ \vdots & \vdots & & \vdots \\ N_s(C) & N_{s+1}(C) & \cdots & N_{2s-1}(C) \end{pmatrix}$$

and \mathbf{N} is the matrix whose first k columns are those of \mathbf{H} and whose last $r - k$ columns are those of \mathbf{H}' .

Note that, by Theorem 4.2, the number of distinct eigenvalues of G is the size of the largest nonsingular Hankel matrix \mathbf{H} described in Theorem 4.4. This is the case since any closed pseudo walk matrix $\mathbf{W}_{\mathbf{v}}$, where \mathbf{v} is any vector presented in Theorem 4.1, has the same rank as $\mathbf{H} = \mathbf{W}_{\mathbf{v}}^T \mathbf{W}_{\mathbf{v}}$.

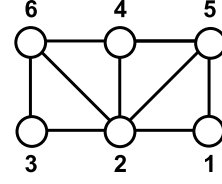
Furthermore, if G has n distinct eigenvalues, then Theorem 4.4 computes the characteristic polynomial of G , and hence is an alternative to the Harary-Sachs coefficient theorem. Almost all graphs have a trivial automorphism group [6]; moreover, such graphs must have n distinct eigenvalues [12]. Thus, almost all graphs may utilize Theorem 4.4 to evaluate coefficients of their characteristic polynomial.

A strongly regular graph with parameters (n, ρ, σ, τ) is a regular graph of degree $\rho \in \{1, 2, \dots, n-2\}$ in which any two adjacent vertices have σ common neighbours and any two non-adjacent vertices have τ common neighbours. A graph is strongly regular if and only if it has exactly 3 distinct eigenvalues [15]; moreover, the parameters ρ , σ and τ may be derived from these 3 eigenvalues. By Theorem 4.2, any closed pseudo walk matrix of a graph G has 3 columns if and only if G is a strongly regular graph. Moreover, by Theorem 4.4, the three distinct eigenvalues of any strongly regular graph (and hence, its 4 parameters) may be determined from the number of closed walks of length up to five within the graph.

5. Examples

Consider the graph G depicted below (right). The six distinct eigenvalues of G are $\{3.223, 1, 0.112, -1, -1.527, -1.809\}$. An orthogonal matrix of orthonormal eigenvectors associated with these eigenvalues is the one displayed underneath (left):

$$\mathbf{X} = \begin{pmatrix} 0.3 & -0.5 & -0.483 & 0.5 & 0.131 & -0.4 \\ 0.566 & 0 & -0.185 & 0 & -0.683 & 0.424 \\ 0.3 & 0.5 & -0.483 & -0.5 & 0.131 & -0.4 \\ 0.424 & 0 & 0.683 & 0 & -0.185 & -0.566 \\ 0.4 & -0.5 & 0.131 & -0.5 & 0.483 & 0.3 \\ 0.4 & 0.5 & 0.131 & 0.5 & 0.483 & 0.3 \end{pmatrix}$$



Let us first determine a pseudo walk matrix $\mathbf{W}_{\mathbf{v}_1}$ such that the Gram matrix of the columns of $\mathbf{W}_{\mathbf{v}_1}$ contains the number of walks in G starting from vertex 1 and ending at vertex 2. The set S_1 under consideration is simply $\{(1, 2)\}$. By Theorem 3.1, a suitable walk vector \mathbf{v}_1 is determined by first constructing the vector \mathbf{d}_1 , whose entries may be taken to be, respectively: $\sqrt{0.3 \times 0.566} = 0.412$, $\sqrt{-0.5 \times 0} = 0$, $\sqrt{-0.483 \times -0.185} = 0.299$, $\sqrt{0.5 \times 0} = 0$, $\sqrt{0.131 \times -0.683} = 0.412i$, $\sqrt{-0.4 \times 0.424} = 0.299i$. Then the walk vector \mathbf{v}_1 is simply $\mathbf{X}\mathbf{d}_1$, which is equal to

$$\mathbf{v}_1 = (-0.021 - 0.126i \quad 0.178 - 0.029i \quad -0.021 - 0.126i \quad 0.379 - 0.289i \quad 0.204 + 0.268i \quad 0.204 + 0.268i)^\top.$$

This walk vector produces the following pseudo walk matrix of rank 4, having complex entries:

$$\mathbf{W}_{\mathbf{v}_1} = \begin{pmatrix} -0.021 - 0.126i & 0.382 + 0.238i & 1.281 - 0.448i & 4.133 + 0.836i \\ 0.178 - 0.029i & 0.745 - 0.004i & 2.420 + 0.096i & 7.802 - 0.307i \\ -0.021 - 0.126i & 0.382 + 0.238i & 1.281 - 0.448i & 4.133 + 0.836i \\ 0.379 - 0.289i & 0.586 + 0.506i & 1.816 - 0.891i & 5.845 + 1.576i \\ 0.204 + 0.268i & 0.536 - 0.444i & 1.712 + 0.740i & 5.517 - 1.244i \\ 0.204 + 0.268i & 0.536 - 0.444i & 1.712 + 0.740i & 5.517 - 1.244i \end{pmatrix}.$$

The Gram matrix of the columns of $\mathbf{W}_{\mathbf{v}_1}$ is

$$\begin{pmatrix} 0 & 1 & 1 & 7 \\ 1 & 1 & 7 & 16 \\ 1 & 7 & 16 & 63 \\ 7 & 16 & 63 & 183 \end{pmatrix}.$$

The entry in the i^{th} row and j^{th} column of this matrix is the number of walks of length $i + j - 2$ starting from vertex 1 and ending at vertex 2 in G , as can be directly verified.

Let us now obtain a pseudo walk matrix $\mathbf{W}_{\mathbf{v}_2}$ for the set $S_2 = \{(1, 1), (2, 2)\}$. This time, the Gram matrix of the columns of $\mathbf{W}_{\mathbf{v}_2}$ contains the number of closed walks starting and ending at vertex 1 or 2. By applying Theorem 3.1 again, this time on this set, vector \mathbf{d}_2 may be taken to be $(0.64 \quad 0.583 \quad 0.695 \quad 0.5 \quad 0.5 \quad 0.517)^\top$, by taking the positive square root for all relevant numbers. Thus, a suitable walk vector is

$$\mathbf{v}_2 = \mathbf{X}\mathbf{d}_2 = (-0.2 \quad 0.04 \quad -0.2 \quad 0.166 \quad 0.334 \quad 1.334)^\top.$$

This walk vector results in the pseudo walk matrix $\mathbf{W}_{\mathbf{v}_2}$ of rank 6. The Gram matrix of the columns of $\mathbf{W}_{\mathbf{v}_2}$ is a Hankel matrix with first row $(2 \quad 0 \quad 7 \quad 10 \quad 51 \quad 132)$ and last row $(132 \quad 478 \quad 1450 \quad 4826 \quad 15288 \quad 49727)$. The entries of these two rows can be confirmed to be the number of closed walks of length $0, \dots, 5$ and of length $5, \dots, 10$ starting and ending at vertex 1 or 2 respectively.

We now determine a walk vector for the set $S = \{(1, 1), (1, 2), (2, 1), (2, 2)\}$. Clearly $S = S_1 \cup S_2 \cup \{(2, 1)\}$. Moreover, \mathbf{v}_1 may be taken to be a walk vector associated with the set $\{(2, 1)\}$ as well. Thus, by Corollary 3.1, a suitable walk vector for S would be $\mathbf{X}\mathbf{d}$, where, for all i , the i^{th} entry of \mathbf{d} is the positive or negative square root of

$$[\mathbf{X}^\top \mathbf{v}_1]_i^2 + [\mathbf{X}^\top \mathbf{v}_2]_i^2 + [\mathbf{X}^\top \mathbf{v}_2]_i^2.$$

If we take the positive square root for all 6 entries of \mathbf{d} , then we obtain the walk vector

$$\mathbf{v} = (0 \quad 0 \quad 0 \quad 0.707 \quad 0.207 \quad 1.207)^\top.$$

However, if we take the positive square root for the first, second and fourth entries for \mathbf{d} , while we take the negative square root for the other entries, then we obtain the alternative walk vector $\mathbf{v}' = (1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0)^\top$, which, of course, is an obvious choice for S .

By Theorem 4.1, one walk vector for a closed pseudo walk matrix associated with $C = \{(v, v) \mid v \in \{1, 2, 3, 4, 5, 6\}\}$ is the sum of the columns of \mathbf{X} , that is, $(-0.452 \quad 0.122 \quad -0.452 \quad 0.355 \quad 0.313 \quad 2.313)^\top$. This results in a closed pseudo

walk matrix of rank 6, confirming Theorem 4.2. The Gram matrix \mathbf{H} of the columns of this closed walk matrix has first row $(6 \ 0 \ 18 \ 24 \ 126 \ 320)$ and last row $(320 \ 1170 \ 3528 \ 11782 \ 37248 \ 121298)$, which can be verified as being the number of all closed walks of length $0, \dots, 5$ and of length $5, \dots, 10$ in G respectively. Furthermore, by applying Theorem 4.4, the coefficients of the minimal polynomial of G , in descending powers of x , are $1, 0, -9, -8, 9, 8$ and -1 . Since all eigenvalues of G are distinct, these are actually the coefficients of the characteristic polynomial of G , as can be verified by inspection.

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