Cycle Spaces of Digraphs

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Abstract

The cycle space of a graph corresponds to the kernel of an incidence matrix. We investigate an analogous subspace for digraphs. In the case of digraphs of graphs, where every edge is replaced by two oppositely directed arcs, we give a combinatorial description of a basis of such a space. We are motivated by a connection to the transition matrices of discrete-time quantum walks.

1 Introduction

The spectrum of a graph is a graph invariant; isomorphic graphs have the same eigenvalues. The natural follow-up problem is to find classes of graphs in which the spectrum determines the graph, see for example [13]. The authors of [2, 13] suggest that the portion of graphs on \( n \) vertices which are determined by their spectrum goes to 1 as \( n \) tends to infinity. It is well-known that any two co-parametric strongly regular graphs are cospectral, so it would seem that spectra may not be the right tool to solving Graph Isomorphism in the class of strongly regular graphs. However, there are many proposed algorithms for Graph Isomorphism for the class of strongly regular graphs, which are based on the spectrum of a matrix associated with the graph, see for example [1, 6]. These algorithms are surprisingly successful on small strongly regular graphs. One such proposed routine is that of Emms et al [4, 5], which is based on the transition matrix of a discrete-time quantum walk in the arc-reversal model, introduced by Kendon in [10]. Many classes of strongly regular graphs on were distinguished by this graph invariant and only one pair of counterexamples is known [7].

In the course of trying to find an infinite family of counterexamples for the above procedure, the authors were led to the study of a directed version of the cycle space of a graph. We find a decomposition of the vector space indexed by the arcs of a graph, with the goal of using it to diagonalize matrices indexed by the arcs of graph. The relation between discrete-time quantum walks and Ihara zeta function was observed in [11]. The positive support of the transition matrix is related to the Bass-Hashimoto edge adjacency operator.

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We proceed with a few basic definitions. The diagraph of a graph $G$ is obtained from $G$ by replacing each edge $\{x, y\}$ with directed edges $xy$ and $yx$. In this article, we study a related kernel $\ker(D_t) \cap \ker(D_h)$, for $X$ a diagraph of a graph $G$. We are interested in its dimension and descriptions of the combinatorial objects in this space.

Let $X$ be a diagraph without loops or parallel arcs. Let $A$ the adjacency matrix of $X$. We consider the following incidence matrices of $X$, both with rows indexed by the vertices of $X$ and columns indexed by the arcs of $X$:

$$(D_h)_{i,j} = \begin{cases} 
1, & \text{if } i \text{ is the head of arc } j; \\
0, & \text{otherwise},
\end{cases}$$

and

$$(D_t)_{i,j} = \begin{cases} 
1, & \text{if } i \text{ is the tail of arc } j; \\
0, & \text{otherwise}.
\end{cases}$$

Let $B(X) = D_t + D_h$ and $N(X) = D_t - D_h$. We will write $N$ and $B$ for simplicity, when the choice of digraph is clear.

In this paper, we find the following main result.

**1.1 Theorem.** For $X$ the diagraph of a graph $G$ with $m$ edges, the subspace $\ker(D_t) \cap \ker(D_h)$ of $\mathbb{R}^{2m}$ has dimension $2m - 2n + b + c$, where $b$ is the number of bipartite components of $X$ and $c$ is the number of components of $X$.

In the case that $G$ is a bipartite graph, we can give an explicit basis of $\ker(D_t) \cap \ker(D_h)$ in terms of the cycle space of $G$.

## 2 Preliminaries

Given a graph $X$, there are two incidence matrices of $X$, which are commonly studied. We will follow the notation and definitions in [8]. For an orientation $X^\sigma$ of $X$, they are given as follows:

$$B(X) = D_h(X^\sigma) + D_t(X^\sigma)$$

and

$$N(X^\sigma) = D_t(X^\sigma) - D_h(X^\sigma),$$

where $D_t(X^\sigma)$ and $D_h(X^\sigma)$ are the tails and heads incidence matrices of $X^\sigma$.

**2.1 Theorem. (Theorem 8.2.1, [8])** For a graph $X$ on $n$ vertices with $b$ bipartite components, the incidence matrix $B(X)$ has rank equal to $n - b$.

It is apparent from the definition that any choice of orientation gives the same incidence matrix $B(X)$. The following theorem implies the choice of orientation does not affect that rank of $N(X^\sigma)$.
2.2 Theorem. (Theorem 8.3.1, [8]) For a graph $X$ on $n$ vertices with $c$ components and an orientation $X^\sigma$ of $X$, the incidence matrix $N(X^\sigma)$ has rank equal to $n - c$.

The kernel of $N(X^\sigma)$ is called the flow space or cycle space and has a combinatorial description in terms of the cycles of the graph. Let $C$ be a cycle in $X$; that is, $C$ is a set of directed edges of $X$ such that if $uv \in C$ then $vu \not\in C$ and $C$ induces a cycle in $X$, when the directions are forgotten. With respect to an orientation $X^\sigma$ of $X$, the signed characteristic vector of $C$ in $C_{m}$ is as follows:

$$(v_C)_{uv} = \begin{cases} 1, & \text{if } uv \in C; \\ -1, & \text{if } vu \in C; \\ 0, & \text{otherwise}. \end{cases}$$

Note that for each directed edge $uv$ of $C$, exactly one of $uv$ and $vu$ appear as a directed edge of $X^\sigma$.

2.3 Theorem. (Corollary 14.2.3, [8]) For a graph $X$ with an orientation $X^\sigma$ of $X$, the flow space $\ker(N(X^\sigma))$ is spanned by the signed characteristic vectors of its cycles.

3 Main result

3.1 Theorem. For $X$ the digraph of a graph $G$ on $n$ vertices and $m$ edges, the subspace $\ker(D_t(X)) \cap \ker(D_h(X))$ of $\mathbb{R}^{2m}$ is

$$\left\{ H \begin{pmatrix} v \\ w \end{pmatrix} \mid v \in \ker(B(X^\sigma)), \ w \in \ker(N(X^\sigma)) \right\},$$

where

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ I & -I \end{pmatrix},$$

and thus has dimension $2m - 2n + b + c$, where $b$ is the number of bipartite components of $X$ and $c$ is the number of components of $X$.

Proof. First observe the following:

$$\ker(D_t(X)) \cap \ker(D_h(X)) = \ker \begin{pmatrix} D_t(X) \\ D_h(X) \end{pmatrix}.$$

We consider $X^\sigma$, any orientation of $G$. Let the edges of $X^\sigma$ be $\{e_1, \ldots, e_m\}$. We order the edges of $X$ as $\{e_1, \ldots, e_m, \bar{e}_1, \ldots, \bar{e}_m\}$ where if $e_i = uv$ then $\bar{e}_i = vu$. We have that

$$D_t(X) = \begin{pmatrix} D_t(X^\sigma) & D_h(X^\sigma) \end{pmatrix} \quad \text{and} \quad D_h(X) = \begin{pmatrix} D_h(X^\sigma) & D_t(X^\sigma) \end{pmatrix}.$$

Thus

$$\begin{pmatrix} D_t(X) \\ D_h(X) \end{pmatrix} = \begin{pmatrix} D_t(X^\sigma) & D_h(X^\sigma) \\ D_h(X^\sigma) & D_t(X^\sigma) \end{pmatrix}. $$
We see that
\[
H \begin{pmatrix} D_t(X) & D_h(X) \\ D_h(X) & D_t(X) \end{pmatrix} H = \begin{pmatrix} D_t(X) + D_h(X) & 0 \\ 0 & D_h(X) - D_t(X) \end{pmatrix} = \begin{pmatrix} B(X) & 0 \\ 0 & N(X) \end{pmatrix}
\]
where
\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ I & -I \end{pmatrix}
\]
and \(H^T = H^{-1} = H\). We have that
\[
\ker \begin{pmatrix} B(X) & 0 \\ 0 & N(X) \end{pmatrix} = \left\{ \begin{pmatrix} v \\ w \end{pmatrix} \mid v \in \ker(B(X)), w \in \ker(N(X)) \right\}.
\]
For \(v \in \ker(B(X))\) and \(w \in \ker(N(X))\), we consider the vector \(H \begin{pmatrix} v \\ w \end{pmatrix}\):
\[
\begin{pmatrix} D_t(X) \\ D_h(X) \end{pmatrix} H \begin{pmatrix} v \\ w \end{pmatrix} = H \begin{pmatrix} B(X) & 0 \\ 0 & N(X) \end{pmatrix} HH \begin{pmatrix} v \\ w \end{pmatrix} = 0
\]
Thus,
\[
\ker \begin{pmatrix} D_t(X) \\ D_h(X) \end{pmatrix} = \left\{ H \begin{pmatrix} v \\ w \end{pmatrix} \mid v \in \ker(B(X)), w \in \ker(N(X)) \right\}
\]
and
\[
\dim \ker(D_t(X)) \cap \ker(D_h(X)) = 2m - 2n + c + b.
\]
as claimed.

When \(G\) is bipartite, there is a natural choice of an orientation, which, together with the matrix of similarity, gives an explicit basis for \(L\).

With respect to \(X^\sigma\), we define two characteristic vectors \(y_C\) and \(w_C\) of \(C\) in \(\mathbb{C}^{2m}\) as follows:
\[
(y_C)_{uv} = \begin{cases} v_{uv}, & \text{if } uv \in E(X^\sigma); \\ -v_{uv}, & \text{otherwise} \end{cases}
\]
and
\[
(w_C)_{uv} = \begin{cases} v_{uv}, & \text{if } uv \in E(X^\sigma); \\ v_{uv}, & \text{otherwise}. \end{cases}
\]
See Figure 1.

3.2 Theorem. Let \(X\) be a bipartite graph, \(X^\sigma\) be an orientation of \(X\), and \(C\) be a cycle basis of \(X\). The subspace \(\dim \ker(D_t(X)) \cap \ker(D_h(X))\) of \(\mathbb{C}^{2m}\) has the following basis:
\[
\{ y_C, w_C \mid C \in \mathcal{C} \}.
\]
Figure 1: Vectors $y_C$ and $w_C$ for a 4-cycle.

**Proof.** We take $X^\sigma$ to be the orientation of $X$ with bipartition $(Y, Z)$ to have all directed edges of $X$ with tails in $Y$ and heads in $Z$. Let $R$ be the $n \times n$ diagonal matrix with entries

$$R_{v,v} = \begin{cases} 1, & \text{if } v \in Y; \\ -1, & \text{if } v \in Z. \end{cases}$$

We see that $RB(X^\sigma) = N(X^\sigma)$.

Let $v \in \ker(N(X^\sigma))$. Since $N(X^\sigma)v = 0$, we have that $RB(X^\sigma)v = 0$. Since $R$ is an invertible matrix, we have that $v \in \ker(B(X^\sigma))$ and so $\ker(N(X^\sigma)) \subseteq \ker(B(X^\sigma))$. Since $R^2 = I$, we also have $RN(X^\sigma) = B(X^\sigma)$ and can similarly show that $\ker(B(X^\sigma)) \subseteq \ker(N(X^\sigma))$, and so $\ker(N(X^\sigma)) = \ker(B(X^\sigma))$.

Theorem 3.1 gives us that

$$\ker \left( \begin{array}{c} D_t(X) \\ D_h(X) \end{array} \right) = \left\{ H \begin{pmatrix} v \\ w \end{pmatrix} \mid v, w \in \ker(N(X^\sigma)) \right\}.$$ 

Observe that

$$\left\{ H \begin{pmatrix} v \\ 0 \end{pmatrix}, H \begin{pmatrix} 0 \\ v \end{pmatrix} \mid v \in \ker(N(X^\sigma)) \right\}$$

is an independent set of vectors in $\ker \left( \begin{array}{c} D_t(X) \\ D_h(X) \end{array} \right)$ whose cardinality is equal to the dimension of $\ker \left( \begin{array}{c} D_t(X) \\ D_h(X) \end{array} \right)$ and is hence a basis. Consider $v \in \ker(N(X^\sigma))$. We see that

$$H \begin{pmatrix} v \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} v \\ v \end{pmatrix}$$

and

$$H \begin{pmatrix} 0 \\ v \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} v \\ -v \end{pmatrix}.$$ 

If $v$ is the characteristic vector of a cycle $C$ in $X^\sigma$, then $\begin{pmatrix} v \\ v \end{pmatrix} = w_C$ and $\begin{pmatrix} v \\ -v \end{pmatrix} = y_C$.  

5
4 Relation to quantum walks

A discrete quantum walk is a process on a graph $G$ governed by a unitary matrix, $U$, which is called the transition matrix. For $uv$ and $wx$ arcs in the digraph of $X$, the transition matrix is defined to be:

$$U_{wx,uv} = \begin{cases} 
\frac{2}{d(v)} & \text{if } v = w \text{ and } u \neq x, \\
\frac{2}{d(v)} - 1 & \text{if } v = w \text{ and } u = x, \\
0 & \text{otherwise.}
\end{cases}$$

We may write this in terms of the incidence matrices of $X$, the digraph of $G$. To describe the quantum walk, we need one more matrix: let $P$ be a permutation matrix with row and columns indexed by the arcs of $D$ such that,

$$P_{wx,uv} = \begin{cases} 
1 & \text{if } x = u \text{ is the tail of arc } w = v \\
0 & \text{otherwise.}
\end{cases}$$

Then, we see that $D_h D_t^T = A(G)$, the adjacency matrix of $G$, and

$$(D_t^T D_h)_{wx,uv} = \begin{cases} 
1 & \text{if } v = w, \\
0 & \text{otherwise.}
\end{cases}$$

If $G$ is regular with valency $k$, we have that

$$U = \frac{2}{k} D_t^T D_h - P.$$ 

It is important to note that $U$ is a $nk \times nk$ unitary matrix. In addition, from the definitions of $D_h$, $D_t$ and $P$, we easily see the following:

$$D_h D_h^T = kI, D_t D_t^T = kI, D_h P = D_t, \text{ and } D_t P = D_h.$$ 

In [9], we prove that one can diagonalize $U$ and related matrices over $\mathbb{C}^{kn}$ by decomposing $\mathbb{C}^{kn} = K \oplus L$, where $K = \text{col}(D_h) \oplus \text{col}(D_t)$ and $L = \text{ker}(D_t) \cap \text{ker}(D_h)$.

5 Further applications

The Bass-Hashimoto edge adjacency matrix $T(G)$ of a graph $G$ is a matrix indexed by end arcs of $G$ such that

$$T(G)_{uv,wx} = \begin{cases} 
1, & \text{if } v = w \text{ and } u \neq x; \\
0, & \text{otherwise.}
\end{cases}$$

The Bass-Hashimoto edge adjacency matrix has been studied in the context of the Ihara zeta function of graphs. [add citations here] Observe that we can write $T(G)$ in terms of incidence matrices as follows:

$$T(G) = D_h^T D_t - P,$$
where $P$ is the permutation matrix taking each arc to the reverse arc. When the context is clear, we will write $T$ for $T(G)$.

An eigenvalue is said to be semi-simple if its algebraic and geometric multiplicities are equal. A matrix is semi-simple if all of its eigenvalues are semi-simple. In [3], the authors find that $T$ is semi-simple over $\ker(D_t(X)) \cap \ker(D_h(X))$ but can fail to be semi-simple in general. In particular, they show that $T$ is not semi-simple if $T$ has a vertex of degree 1 and they ask if the presence of vertices of degree 1 are the only obstructions to simplicity. Here, we give an answer in the negative by computation, but find that $T$ is semi-simple for regular graphs of degree at least 2.

We find, by a computation using Sage [12], that for graphs on $n$ vertices where $n = 1, \ldots, 6$ the only graphs for which the Bass-Hashimoto edge adjacency matrix has a non-semi-simple eigenvalue have a vertex of degree 1. However, the statement is false for graphs on 7 vertices; there are 2 graphs which have $(x^2 + x + 2)^2$ as a factor of the minimal polynomial of $T$ and so the roots of $(x^2 + x + 2)^2$ are non-semi-simple eigenvalues. For graphs on 8 vertices, there are 52 graphs which have a non-semi-simple eigenvalue and which contain no vertex of degree 1. Of these graphs 22 have $x^2 + 2$ as a repeated root of the minimal polynomial of $T$ and 30 have $x^2 + x + 2$ as a repeated root of the minimal polynomial of $T$. Figure 2 shows an example of one such graph; it is connected with a connected complement, has no vertex of degree 1, and its minimal polynomial of $T$ is

$$(x - 1)(x + 1)(x^2 + 3)(x^2 + 4)(x^2 + 2)^2(x^7 + x^6 - 2x^5 - 14x^4 - 39x^3 - 59x^2 - 72x - 72).$$

![Figure 2: A graph on 8 vertices with two non-semi-simple eigenvalues and no vertex of degree 1.](image)

In relation to discrete-time quantum walks, the authors of [4] study the positive support of the transition matrix $U$; they study the matrix $S^+(U)$ whose $(i,j)$ entry is 1 whenever
the \((i,j)\) entry of \(U\) is positive, and is 0 otherwise. In terms of incidence matrices, we can write this matrix as follows:

\[
S^+(U) = D^T_i D_h - P.
\]

Observe that

\[
PT(G)P = PD^T_h D_t P - P^3 = D^T_i D_h - P
\]

which implies that \(T(G)\) is similar to \(S^+(U)\) via \(P\) and hence \(T\) and \(S^+(U)\) have the same eigenvalues and, further, an eigenvalue \(\lambda\) of \(T\) is semi-simple if and only if \(\lambda\) is a semi-simple eigenvalue of \(S^+(U)\).

Theorem 3.1 of [9] finds that for \(k\)-regular graphs on \(n\) vertices with \(k \geq 2\), \(S^+(U)\) is diagonalizable over \(\mathbb{C}^kn\) and find the eigenvalues by showing that \(L\) and \(K\) are \(S^+(U)\)-invariant and diagonalizing over each space separately. This gives the immediately corollary.

5.1 Corollary. The Bass-Hashimoto edge adjacency matrix \(T\) is semi-simple for all \(k\)-regular graphs with \(k \geq 2\).

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