ON THE DIGRAPH OF A UNITARY MATRIX

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Abstract. Given a matrix $M$ of size $n$, the digraph $D$ on $n$ vertices is said to be the digraph of $M$, when $M_{ij} \neq 0$ if and only if $(v_i, v_j)$ is an arc of $D$. We give a necessary condition, called strong quadrangularity, for a digraph to be the digraph of a unitary matrix. With the use of such a condition, we show that a line digraph, $\overrightarrow{L}D$, is the digraph of a unitary matrix if and only if $D$ is Eulerian. It follows that, if $D$ is strongly connected and $\overrightarrow{L}D$ is the digraph of a unitary matrix then $\overrightarrow{L}D$ is Hamiltonian. We conclude with some elementary observations. Among the motivations of this paper are coined quantum random walks, and, more generally, discrete quantum evolution on digraphs.

1. Introduction

Let $D = (V, A)$ be a digraph on $n$ vertices, with labelled vertex set $V(D)$, arc set $A(D)$ and adjacency matrix $M(D)$. We assume that $D$ may have loops and multiple arcs. Let $M$ be a matrix over any field. A digraph $D$ is the digraph of $M$, or, equivalently, the pattern of $M$, if $|V(D)| = n$, and, for every $v_i, v_j \in V(D)$, $(v_i, v_j) \in A(D)$ if and only if $M_{ij} \neq 0$. The support $sM$ of the matrix $M$ is the $(0, 1)$-matrix with element

$$s_{M_{ij}} = \begin{cases} 1 & \text{if } M_{ij} \neq 0, \\ 0 & \text{otherwise}. \end{cases}$$

Then the digraph of a matrix is the digraph whose adjacency matrix is the support of the matrix. The line digraph of a digraph $D$, denoted by $\overrightarrow{L}D$, is the digraph whose vertex set $V(\overrightarrow{L}D)$ is $A(D)$ and $((v_i, v_j), (v_j, v_k)) \in A(\overrightarrow{L}D)$ if and only if $(v_i, v_j), (v_j, v_k) \in A(D)$.

A discrete quantum random walk on a digraph $D$ is a discrete walk on $D$ induced by a unitary transition matrix. The term quantum random walk was coined by Gudder (see, e.g., [G88]), who introduced the model and proposed to use it to describe the motion of a quantum object in discrete space-time and to describe the internal dynamics of elementary particles. Recently, quantum random walks have been rediscovered, in the context of quantum computation, by Ambainis et al. (see [ABNVW01] and [AKV01]). Since the notion of quantum random walks is analogous to the notion of random walks, interest on quantum random walks has been fostered by the successful use of random walks on combinatorial structures in probabilistic algorithms (see, e.g., [93]). Clearly, a quantum random walk on a digraph $D$ can be defined if and only if $D$ is the digraph of a unitary matrix. Inspired by the work of David Meyer on quantum cellular automata [M96], the authors of [ABNVW01] and [AKV01] overcame this obstacle in the following way. In order to define a quantum random walk on a simple digraph $D$, which is regular and is not the digraph of a unitary matrix, a quantum random walk on $\overrightarrow{L}D$ is defined. The digraph $\overrightarrow{L}D$ is the digraph of a unitary matrix. When we chose an appropriate labeling

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for $V(\overrightarrow{L}D)$, a quantum random walk on $\overrightarrow{L}D$ induces a probability distribution on $V(D)$. The quantum random walk on $\overrightarrow{L}D$ is called the coined quantum random walk on $D$.

With this scenario in mind, the question which this paper addresses is the following: On which digraphs can quantum random walks be defined? In a more general language, we are interested in the combinatorial properties of the digraphs of unitary matrices. We give a simple necessary condition, called strong quadrangularity, for a digraph to be digraph of a unitary matrix. While it seems too daring to conjecture that such a condition is sufficient in the general case, we discover “accidentally” that strong quadrangularity is sufficient when the digraph is a line digraph. We also prove that if a line digraph of a strongly connected digraph is the digraph of a unitary matrix, then it is Hamiltonian. We observe that strong quadrangularity is sufficient to show that certain strongly regular graphs are digraphs of unitary matrices and that $n$-paths, $n$-cycles, directed trees and trees are not. In [GZ98] and [M96] the fact that an $n$-path is not the digraph of a unitary matrix was called the NO-GO Lemma. A consequence of the lemma was that there is no nontrivial, homogeneous, local, one-dimensional quantum cellular automaton. Proposition 4 below can be then interpreted as a simple combinatorial version of the NO-GO Lemma.

We refer to [TS91] and to [BR91], for notions of graph theory and matrix theory, respectively.

2. Digraphs of unitary matrices

Let $D = (V, A)$ be a digraph. A vertex of a digraph is called source (sink) if it has no ingoing (outgoing) arcs. A vertex of a digraph is said to be isolated if it is not joined to another vertex. We assume that $D$ has no sources, sinks and disconnected loopless vertices. By this assumption, $A(D)$ has neither zero-rows nor zero-columns. For every $S \subseteq V(D)$, denote by

$N^+ [S] = \{ v_j : (v_i, v_j) \in A(D), v_i \in S \}$ \quad and \quad $N^- [S] = \{ v_i : (v_i, v_j) \in A(D), v_j \in S \}$

the out-neighbourhood and in-neighbourhood of $S$, respectively. Denote by $|X|$ the cardinality of a set $X$. The non-negative integers $|N^-[v_i]|$ and $|N^+[v_i]|$ are called invalency and outvalency of the vertex $v_i$, respectively. A digraph $D$ is Eulerian if and only if every vertex of $D$ has equal invalency and outvalency.

The notion defined in Definition 1 is standard in combinatorial matrix theory (see, e.g., [BR91]). In graph theory, the term quadrangular was first used in [GZ98].

**Definition 1.** A digraph $D$ is said to be quadrangular if, for any two distinct vertices $v_i, v_j \in V(D)$, we have

$|N^+[v_i] \cap N^+[v_j]| \neq 1 \quad$ and \quad $|N^-[v_i] \cap N^-[v_j]| \neq 1$.

**Definition 2.** A digraph $D$ is said to be strongly quadrangular if there does not exist a set $S \subseteq V(D)$ such that, for any two distinct vertices $v_i, v_j \in S$,

$N^+[v_i] \cap \bigcup_{j \neq i} N^+[v_j] \neq \emptyset \quad$ and \quad $N^+[v_i] \cap N^+[v_j] \subseteq T$,

where $|T| < |S|$, and similarly for the in-neighbourhoods.

**Remark 1.** Note that if a digraph is strongly quadrangular then it is quadrangular.

**Lemma 1.** Let $D$ be a digraph. If $D$ is the digraph of a unitary matrix then $D$ is strongly quadrangular.

**Proof.** Suppose that $D$ is the digraph of a unitary matrix $U$ and that $D$ is not strongly quadrangular. Then there is a set $S \subseteq V(D)$ such that, for any two distinct vertices $v_i, v_j \in S$, $N^+[v_i] \cap \bigcup_{j \neq i} N^+[v_j] \neq \emptyset$ and $N^+[v_i] \cap N^+[v_j] \subseteq T$ where $|T| < |S|$. This implies that in $U$, there is a set $S'$ of rows which contribute, with at least one nonzero entry, to the inner product with some other rows in $S'$. In addition, the nonzero entries of any two distinct rows in $S'$,
which contribute to the inner product of the two rows, are in the columns of the same set of columns $T'$ such that $|T'| < |S'|$. Then the rows of $S'$ form a set of orthonormal vectors of dimension smaller than the cardinality of the set itself. This contradicts the hypothesis. The same reasoning holds for the columns of $U$. 

Two digraphs $D$ and $D'$ are permutation equivalent if there are permutation matrices $P$ and $Q$, such that $M(D') = PM(D)Q$ (and hence also $P^{-1}M(D')Q^{-1} = M(D)$). If $Q = P^{-1}$, then $D$ and $D'$ are said to be isomorphic. We write $D \cong D'$ if $D$ and $D'$ are isomorphic. Denote by $I_n$ the identity matrix of size $n$. Denote by $A^T$ the transpose of a matrix $A$.

**Lemma 2.** Let $D$ and $D'$ be permutation equivalent digraphs. Then $D$ is the digraph of a unitary matrix if and only if $D'$ is.

**Proof.** Suppose that $D$ is the digraph of a unitary matrix $U$. Then, for permutation matrices $P$ and $Q$, we have $PUQ = U'$, where $U'$ is a unitary matrix of the digraph $D'$. The converse is similar. 

**Lemma 3.** For any $n$ the complete digraph is the digraph of a unitary matrix.

**Proof.** The lemma just means that for every $n$ there is a unitary matrix without zero entries. An example is given by the Fourier transform on the group $\mathbb{Z}/n\mathbb{Z}$ (see, e.g., [199]).

A digraph $D$ is said to be $(k, l)$-regular if, for every $v_i \in V(D)$, $|N^{-}\{v_i\}| = k$ and $|N^{+}\{v_i\}| = l$. If $k = l$ then $D$ is said to be simply $k$-regular.

**Remark 2.** Not every $k$-regular digraph is the digraph of a unitary matrix. Let

$$M(D) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$ 

Note that $D$ is 2-regular and it is not quadrangular.

**Remark 3.** Not every quadrangular digraph is the digraph of a unitary matrix. Let

$$M(D) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}.$$ 

Note that $D$ is quadrangular and is not the digraph of a unitary matrix. In fact, $D$ is not strongly quadrangular.

**Definition 3.** A digraph $D$ is said to be specular when, for any two distinct vertices $v_i, v_j \in V(D)$, if $N^{+}\{v_i\} \cap N^{+}\{v_j\} \neq \emptyset$, then $N^{+}\{v_i\} = N^{+}\{v_j\}$, and, equivalently, if $N^{-}\{v_i\} \cap N^{-}\{v_j\} \neq \emptyset$ then $N^{-}\{v_i\} = N^{-}\{v_j\}$.

**Definition 4.** A $n \times m$ matrix $M$ is said to have independent submatrices $M_1$ and $M_2$ when, for every $1 \leq i, k \leq n$ and $1 \leq j, l \leq m$, if $M_{ij} \neq 0$ is an entry of $M_1$ and $M_{kl} \neq 0$ is an entry of $M_2$ then $i \neq k$ and $j \neq l$.

**Theorem 1.** A specular and strongly quadrangular digraph is the digraph of a unitary matrix.

**Proof.** Let $D$ be a digraph. Note that if $D$ is specular and strongly quadrangular then $M(D)$ is composed of independent matrices. The theorem follows then from Lemma 3.

The following theorem collects some classic results on line digraphs (see, e.g., [199]).

**Theorem 2.** Let $D$ be a digraph.
(i) Then, for every $\{v_i, v_j\} \in V(\overrightarrow{L}D)$,
\[ N^+ [\{v_i, v_j\}] = N^+ [v_j] \text{ and } N^- [\{v_i, v_j\}] = N^- [v_i]. \]
(ii) A digraph $D$ is a line digraph if and only if $\overrightarrow{L}D$ is specular.
(iii) Let $D$ be a strongly connected digraph. Then $D$ is Eulerian if and only if $\overrightarrow{L}D$ is Hamiltonian.

**Corollary 1.** A strongly quadrangular line digraph is the digraph of a unitary matrix.

**Proof.** The proof is obtained by point (i) of Theorem 2 together with Theorem 1.

**Remark 4.** Not every line digraph which is the digraph of a unitary matrix is Eulerian. Let
\[ M(D) = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \text{ and } M(\overrightarrow{L}D) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix}. \]
Note that $\overrightarrow{L}D$ is not Eulerian.

In a digraph, a directed path of length $r$, from $v_1$ to $v_{r+1}$, is a sequence of arcs of the form $(v_1, v_2), (v_2, v_3), \ldots, (v_r, v_{r+1})$, where all vertices are distinct. A directed path is an Hamiltonian path if it included all vertices of the digraph. A directed path, in which $v_1 = v_{r+1}$, is called directed cycle. An Hamiltonian path, in which $v_1 = v_{r+1} = v_n$ and $|V(D)| = n$, is called Hamiltonian cycle. A digraph with an Hamiltonian cycle is said to be Hamiltonian.

**Theorem 3.** Let $D$ be a digraph. Then $\overrightarrow{L}D$ is the digraph of a unitary matrix if and only if $D$ is Eulerian or the disjoint union of Eulerian components.

**Proof.** Suppose that $\overrightarrow{L}D$ is the digraph of a unitary matrix. By Corollary 1, $\overrightarrow{L}D$ is strongly quadrangular. If there is $v_i \in V(\overrightarrow{L}D)$ such that $|N^+[v_i]| = 1$ then for every $v_j \in V(\overrightarrow{L}D)$, $N^+[v_i] \cap N^+[v_j] = \emptyset$. Suppose that, for every $v_i \in V(\overrightarrow{L}D)$, $|N^+[v_i]| = 1$. Since $\overrightarrow{L}D$ is strongly quadrangular then $A(D) = A(\overrightarrow{L}D)$ and it is a permutation matrix. In general, for every $v_i \in V(\overrightarrow{L}D)$, if $|N^+[v_i]| = k > 1$, then there is a set $S \subset V(\overrightarrow{L}D)$ with $|S| = k - 1$ and not including $v_i$ such that, for every $v_j \in S$, $N^+[v_j] = N^+[v_i]$. Writing $v_i = uv$, where $u, v \in V(D)$, by Theorem 2 $N^+[v_i] = N^+[v]$. It follows that $|N^+[u]| = k$. Then, because of $S$, it is easy to see that in $A(D)$ there are $k$ arcs with head $w$. Hence $|N^+[v]| = |N^-[v]|$, and $D$ is Eulerian. The proof of the sufficiency is immediate.

**Corollary 2.** Let $D$ be a strongly connected digraph. Let $\overrightarrow{L}D$ be the digraph of a unitary matrix. Then $\overrightarrow{L}D$ is Hamiltonian.

**Proof.** We obtain the proof by point (iii) of Theorem 2 together with Theorem 3.

Let $G$ be a group with generating set $S$. The Cayley digraph of $G$ in respect to $S$ is the digraph denoted by $\text{Cay}(G, S)$, with vertex set $G$ and arc set including $(g, h)$ if and only if there is a generator $s \in S$ such that $gs = h$.

**Corollary 3.** The line digraph of a Cayley digraph is the digraph of a unitary matrix.

**Proof.** The corollary follows from Theorem 3 since a Cayley digraph is regular.
ON THE DIGRAPH OF A UNITARY MATRIX

$r, m > 1$, is denoted by $rK_m$. If $m = 2$ then $rK_2$ is called ladder graph. A strongly regular graph is disconnected if and only if it is isomorphic to $rK_m$.

**Remark 5.** Not every strongly regular graphs is the digraph of a unitary matrix. The graph $srg(10, 3, 0, 1)$ is called Petersen’s graph. It is easy to check that $srg(10, 3, 0, 1)$ is not quadrangular.

**Remark 6.** By Theorem [1], if a digraph $D$ is permutation equivalent to a disconnected strongly quadrangular graph, then $D$ is the digraph of a unitary matrix.

The complement of a digraph $D$ is a digraph denoted by $\overline{D}$ with the same vertex set of $D$ and with two vertices adjacent if and only if the vertices are not adjacent in $D$. A digraph $D$ is self-complementary if $D \cong \overline{D}$.

**Remark 7.** The fact that $D$ is the digraph of a unitary matrix does not imply that $D$ is. The digraph used in the proof of Proposition 2 provides a counterexample. Note that this does not hold in the case where $D$ is self-complementary.

A digraph $D$ is an $n$-path, if $V(D) = \{v_1, v_2, ..., v_n\}$ and

$$A(D) = \{(v_1, v_2), (v_2, v_1), (v_2, v_3), (v_3, v_2), ..., (v_{n-1}, v_n), (v_n, v_{n-1})\},$$

where all the vertices are distinct. An $n$-path, in which $v_1 = v_n$, is called $n$-cycle. A digraph $D$ is a directed $n$-cycle if $A(D) = \{(v_1, v_2), (v_2, v_3), ..., (v_{n-1}, v_1)\}$. A digraph without directed cycles if a directed tree. A graph without cycle is a tree.

**Proposition 1.** Let $D$ be a digraph. If $D$ is permutation equivalent to an $n$-path then it is not the digraph of a unitary matrix.

*Proof.* A digraph is strongly connected if and only if it is the digraph of an irreducible matrix. Since an $n$-path is strongly connected, it is the digraph of an irreducible matrix. Note that the number of arcs of an $n$-path is $2(n - 1)$. The proposition is proved by Lemma 1 together with the following result (see, e.g., [BR91]). Let $M$ be an irreducible matrix of size $n$ and with exactly $2(n - 1)$ nonzero entries. Then there is a permutation matrix $P$, such that

$$PMP^\top = \begin{bmatrix} a_{11} & 0 & \cdots & 0 & 1 \\ 1 & a_{22} & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \ddots & 0 \\ 0 & 0 & \cdots & 1 & a_{nn} \end{bmatrix},$$

where $a_{ii}$ can be equal to zero or one. It is easy to see that for any choice of the diagonal entries the digraph of $PMP^\top$ is not quadrangular.

**Proposition 2.** If a digraph $D$ is permutation equivalent to one of the following digraphs, then $D$ is not the digraph of a unitary matrix: $n$-path with a loop at each vertex, $n$-cycle, directed tree, tree.

*Proof.* Chosen any labeling of $D$, the proposition follows from Lemma 1 and Lemma 2.

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