Graphs of unitary matrices

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Abstract

The *support* of a matrix M is the $(0,1)$-matrix with ij-th entry equal to 1 if the ij-th entry of M is non-zero, and equal to 0, otherwise. The digraph whose adjacency matrix is the support of M is said to be the *digraph of M*. In this paper, we observe some general properties of digraphs of unitary matrices.

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1 Introduction

A (finite) *directed graph*, for short *digraph*, consists of a non-empty finite set of elements called *vertices* and a (possibly empty) finite set of ordered pairs of vertices called *arcs*. Let $D = (V, A)$ be a digraph with vertex-set $V(D)$ and arc-set $A(D)$. In a digraph a *loop* is an arc of the form (v_i, v_i). In a digraph D, if $(v_i, v_j), (v_j, v_i) \in A(D)$ the pair $\{(v_i, v_j), (v_j, v_i)\}$ is called *edge* and denoted simply by $\{v_i, v_j\}$. A digraph D is *symmetric* if, for every $v_i, v_j \in V(D)$, $(v_i, v_j) \in A(D)$ if and only if $(v_j, v_i) \in A(D)$. Naturally, a symmetric digraph is also called *graph*. The *adjacency matrix* of a digraph D on n vertices, denoted by $M(D)$, is the $n \times n$ $(0,1)$-matrix with ij-th entry

$$M_{i,j}(D) = \begin{cases} 1 & \text{if } (v_i, v_j) \in A(D), \\ 0 & \text{otherwise.} \end{cases}$$

Let M be an $n \times n$ matrix (over any field). The *support of M* is the $n \times n$ $(0,1)$-matrix with ij-th entry equal to 1 if $M_{i,j} \neq 0$, and equal to 0, otherwise. The *digraph of M* is the digraph whose adjacency matrix is the support of M. If a digraph D is the digraph of a matrix M then we say that D (or, indistinctly, $M(D)$) *supports* M. An $n \times n$ complex matrix U is *unitary* if $U^{\dagger}U = UU^{\dagger} = I_n$, where $U^{\dagger}$ is the adjoint of U and I_n the identity matrix of size n. We denote by $\mathcal{U}$ the set of the digraphs of unitary matrices. Properties of digraphs of unitary matrices are investigated in [BBS93], [CJLP99], [CS00], [GZ98] and [S03] (see also the references contained therein). These articles mainly study the number

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of non-zero entries in unitary matrices with specific combinatorial properties (*e.g.* irreducibility, first column(row) without zero-entries, *etc.*). The present paper observes some structural properties of digraphs and Cayley digraphs, of unitary matrices. The next two subsections outline the paper.

1.1 Cayley digraphs

Section 2 is dedicated to Cayley digraphs. Let G be a finite group and let $S \subset G$. We denote by e the identity element of a group G. We write $G = \langle S : \mathcal{R} \rangle$ to mean that G is generated by S with a set of relations $\mathcal{R}$. When we do not need to specify $\mathcal{R}$, we write simply $G = \langle S \rangle$.

The *Cayley digraph of G with respect to S*, denoted by $X(G; S)$, is the digraph whose vertex-set is G, and whose arc-set is the set of all ordered pairs $\{(g, sg) : g \in G, s \in S\}$. Let ρ_{reg} be the regular permutation representation of G. Then

$$M(X(G;S)) = \sum_{i=1}^{k} \rho_{reg}(s_i), \quad \text{with} \quad S = \{s_1, s_2, ..., s_k\}.$$

Note that $M(X(G;S)) = \widehat{\delta_S}(\rho_{reg})$, where $\widehat{\delta_S}(\rho_{reg})$ is the Fourier transform at ρ_{reg} of the characteristic function of S. For every $S \subset V(D)$, let $N^-(S) = \{v_i : (v_i, v_j) \in A(D), v_j \in S\}$ and $N^+(S) = \{v_j : (v_i, v_j) \in A(D), v_i \in S\}$ be the *in-neighbourhood* and the *out-neighbourhood* of S, respectively. If D is a graph the *neighbourhood* of S is denoted simply by $N(S)$. A digraph D is *d-regular* if, for every $v_i \in V$, $|N^-(v_i)| = |N^+(v_i)| = d$. A Cayley digraph $X(G;S)$ is on $n = |G|$ vertices and d-regular, where $d = |S|$. If $S = S^{-1}$ then the Cayley digraph $X(G;S)$ is called *Cayley graph*. In Section 2, we prove the following theorem, and construct some examples.

Theorem 1 *Let G be a group with a generating set of two elements. Then there exists a set $S \subset G$, such that $G = \langle S \rangle$ and the Cayley digraph $X(G;S) \in \mathcal{U}$.*

Since every finite simple group has a generating set of two elements [AG84], we have this corollary:

Corollary 2 *Let G be a finite simple group. Then there exists a set $S \subset G$, such that $G = \langle S \rangle$ and the Cayley digraph $X(G;S) \in \mathcal{U}$.*

Let Π_n be the group of all permutation matrices of size n. Let $P, Q \in \Pi_n$. We say that P and Q are *complementary* if, for any $1 \leq h, i, j, k \leq n$,

$$P_{i,j} = P_{h,k} = Q_{i,k} = 1 \quad \text{imply} \quad Q_{h,j} = 1,$$

and, consequently,

$$Q_{i,j} = Q_{h,k} = P_{i,k} = 1 \quad \text{imply} \quad P_{h,j} = 1.$$

We make some observations about Cayley digraphs whose adjacency matrix is sum of complementary permutations. We show that the n-cube is the digraph of a unitary matrix. This is also true for the de Bruijn digraph [ST]. It might be interesting to remark that the n-cube and the de Bruijn digraphs are among the best-known architectures for interconnection networks (see, *e.g.*, [H97], for a survey of this subject, with particular attention to Cayley digraphs). It would be interesting to deepen the study of digraphs of unitary matrices seen as specific architectures for interconnection networks.

1.2 Digraphs

Section 3 is dedicated to digraphs in general. Theorem 3 is the main result of the section. A *dipath* is a non-empty digraph D, where $V(D) = \{v_0, v_1, ..., v_k\}$ and $A(D) = \{(v_0, v_1), (v_1, v_2), ..., (v_{k-1}, v_k)\}$. The vertex v_0 is the *initial vertex* of D; the vertex v_k is the *final vertex*. We say that D is a *dipath from* v_0 *to* v_k. A *path* is a non-empty graph D, with $V(D) = \{v_0, v_1, ..., v_k\}$ and $A(D) = \{\{v_0, v_1\}, \{v_1, v_2\}, ..., \{v_{k-1}, v_k\}\}$. Two or more dipaths (paths) are *independent* if none of them contains an inner vertex of another. A digraph is *connected* if, for every v_i and v_j, there is a dipath from v_i to v_j, or *viceversa*; *strongly-connected* if, for every v_i and v_j, there is a dipath from v_i to v_j and to v_j to v_i. A Cayley digraph is strongly-connected. A k-*dicycle* is a dipath on k arcs in which the initial and final vertex coincide. If all the vertices and the arcs of a dipath (dicycle) are *all* distinct then the dipath (dicycle) is an *Hamilton dipath* (*dicycle*). A digraph spanned by an Hamilton dicycle is said to be *hamiltonian*. In a graph, the analogue of dicycle and hamiltonian dipath (dicycle) are called *cycle* and *hamiltonian path* (*cycle*). In a digraph D on $n \geq 2$ vertices, a *disconnecting set* of arcs (edges) is a subset $T \subset A(D)$ such that $D - T$ has more connected components than D. The *arc(edge)-connectivity* is the smallest number of edges in any disconnecting set. A *cut* of D is a subset $S \subset V(D)$ such that $D - S$ has more connected components than D. The *vertex-connectivity* of D is the smallest number of vertices in any cut of D. A digraph D is said to be k-*vertex-connected* (k-*arc(edge)-connected*) if its vertex-connectivity (arc(edge)-connectivity) is larger or equal than k. A *cut-vertex*, a *directed bridge*, and a *bridge*, are respectively a vertex, an arc, and an edge, whose deletion increases the number of connected components of D. A digraph is *inseparable* if it is without cut-vertices; *bridgeless* if it is without bridges. Let $\overleftrightarrow{K}_2$ and $\overleftrightarrow{K}_2^+$ be respectively the complete graph on two vertices and the complete graph on two vertices with a self-loop at each vertex. We prove the following theorem, and state some of its natural corollaries.

Theorem 3 *Let D be a digraph. If $D \in \mathcal{U}$ then:*

1. *D is without directed bridges;*

2. *D is bridgeless, unless the bridge is in a connected component that is either $\overleftrightarrow{K}_2$ or $\overleftrightarrow{K}_2^+$.*

3. *D is inseparable, unless a cut-vertex is in a connected component that is either $\overleftrightarrow{K}_2$ or $\overleftrightarrow{K}_2^+$.*

1.3 A motivation

Unitary matrices appear in many areas of Physics and are of fundamental importance in Quantum Mechanics. The *time-evolution* of the state of an n-level quantum system, assumed to be isolated from the environment, is reversible and determined by the rubric $\rho \longrightarrow U_t \rho U_t^{-1}$, where $\{U_t : -\infty < t < \infty\}$ is a continuous group of unitary matrices, and ρ, the *state of the system*, is an $n \times n$ Hermitian matrix, which is positive definite and has unit trace. Sometimes it is useful to look at a quantum system as evolving *discretely*, under the same unitary matrix: $\rho \longrightarrow U\rho U^{-1} \longrightarrow U^2 \rho U^{-2} \longrightarrow \cdots \longrightarrow U^n \rho U^{-n}$. Suppose that to an n-level quantum system is assigned a digraph D on n vertices, in the following sense: the vertices of D are labeled by given states of the system; the arc (v_i, v_j) means non-zero probability of transition from the state labeled by v_i to the state labeled by v_j, in one time-step, that is in one application of U. As it happens for random walks on graphs, important features of this evolution depend on the combinatorial properties of D, the digraph of the "transition matrix" U (here U unitary rather than stochastic). Quantum evolution in digraphs have recently drawn attention in Quantum Computation (see *e.g.*, [AAKV01], [SKW02] and [C+03]) and in the study of statistical properties of quantum systems in relation to Random Matrix Theory (see, *e.g.*, [KS99], [T01], [KS03], [ST] and the references contained therein).

2 Cayley digraphs

2.1 Proof of Theorem 1

The *line digraph* of a digraph D, denoted by $\vec{L}D$, is defined as follows: the vertex-set of $\vec{L}D$ is $A(D)$; $(v_i, v_j), (v_k, v_l) \in A\left(\vec{L}D\right)$ if and only if $v_j = v_k$. The digraph D is said to be the *base* of $\vec{L}D$. (See, *e.g.*, [P96], for a survey on line graphs and digraphs.)

Definition 4 (Independent full submatrix) *A rectangular array, say M', of entries from an $n \times n$ matrix M is an* independent full submatrix *when, if $M_{i,j} \in M'$ then, for every $1 \leq k, l \leq n$, either $M_{i,k} \in M'$ or $M_{i,k} = 0$, and, either $M_{l,j} \in M'$ or $M_{l,j} = 0$. In addition, if $M_{i,j} \in M'$ then $M_{i,j} \notin M''$, where M'' is an independent full submatrix different from M'.*

Example 5 *Consider the matrix*

$$M = \begin{bmatrix} 0 & 0 & x_{1,3} & x_{1,4} & x_{1,5} \\ 0 & 0 & x_{2,3} & x_{2,4} & x_{2,5} \\ x_{3,1} & x_{3,2} & 0 & 0 & 0 \\ x_{4,1} & x_{4,2} & 0 & 0 & 0 \\ 0 & 0 & x_{5,3} & x_{5,4} & x_{5,5} \end{bmatrix}.$$

The matrices

$$\begin{bmatrix} x_{3,1} & x_{3,2} \\ x_{4,1} & x_{4,2} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} x_{1,3} & x_{1,4} & x_{1,5} \\ x_{2,3} & x_{2,4} & x_{2,5} \\ x_{5,3} & x_{5,4} & x_{5,5} \end{bmatrix}$$

are independent full submatrices of M.

The following is an easy lemma. This can be also seen as a corollary of Theorem 2.15 in [S03].

Lemma 6 *Let* D *be a Cayley digraph. If there exists a digraph* D' *such that* $D = \overrightarrow{L}D'$ *then* $D \in \mathcal{U}$.

Proof. By the *Richard characterization of line digraphs* (see, *e.g.*, [P96]), a digraph D is a line digraph if and only if the following two conditions hold:

- The columns of $M(D)$ are identical or orthogonal.
- The rows of $M(D)$ are identical or orthogonal.

This means that, if D is a line digraph then every non-zero entry of $M(D)$ belongs to an independent full submatrix. Moreover if D is a regular line digraph then *all* the independent full submatrices of $M(D)$ are square. Suppose that D is a Cayley digraph and a line digraph. Observe that:

(i) Since D is strongly-connected, $M(D)$ has neither zero-rows nor zero-columns.

(ii) Since D is regular, every independent full submatrix of $M(D)$ is square.

Combining (i) and (ii), and since the all-ones matrix supports a unitary matrix, the lemma follows. ■

Let $\mathbb{Z}_n$ be the additive group of the integers modulo n.

Remark 7 *The converse of Lemma 6 is false. For example, consider the Cayley digraph* $D = X(\mathbb{Z}_4; \{1,2,3\})$. *The adjacency matrix of* D *is*

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

The matrix

$$U = \frac{1}{\sqrt{3}} \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & -1 & 1 \\ 1 & 1 & 0 & -1 \\ 1 & -1 & 1 & 0 \end{bmatrix}$$

is unitary. Since $M(D)$ *supports* U, $D \in \mathcal{U}$. *Note that* D *is not a line digraph since it does not satisfy the Richard characterization.*

A *multidigraph* is a digraph with possibly more than one arc (v_i, v_j), for some v_i and v_j.

Lemma 8 (Mansilla-Serra, [MS01]) *Let $G = \langle S \rangle$ be a finite group. If, for some $x \in S^{-1}$, $xS = H$, where H is a subgroup of G such that $|H| = k = |S|$, then $X(G;S) = \overrightarrow{L}D$, where D is a k-regular (multi)digraph.*

Let C_n be a cyclic group of order n. The proof of Theorem 1 makes use of Lemma 6 and Lemma 8.

Proof of Theorem 1. Let $G = \langle S \rangle$, where $S = \{s_1, s_2\}$. Take $s_1^{-1} \in S^{-1}$ (or, equivalently, s_2^{-1}). Then $s_1^{-1}S = \{s_1^{-1}s_1, s_1^{-1}s_2\} = \{e, s_1^{-1}s_2\}$. Let $s_1^{-1}s_2$ have order n. Consider $C_n = \langle s_1^{-1}s_2 \rangle$. Write $T = s_1C_n$. Then $C_n = s_1^{-1}T$. Now, observe that $s_1s_1^{-1}s_2 = s_2$ and $s_1\left(s_1^{-1}s_2\right)^{-1}s_1^{-1}s_2 = s_1s_2^{-1}s_1s_1^{-1}s_2 = s_1$. Then $S \subset T$ and $G = \langle T \rangle$. Since T is a left coset of C_n, $|T| = n = |C_n|$. By Lemma 8, $X(G;T)$ is a line digraph, and hence, by Lemma 6, $X(G;T) \in \mathcal{U}$. ■

2.2 Examples

Let D_n be a dihedral group of order $2n$.

Example 9 *The standard presentation of D_n (see, e.g., [CM72], §1.5) is*

$$\left\langle s_1, s_2 : s_1^n = s_2^2 = e, s_2s_1s_2 = s_1^{-1} \right\rangle.$$

By Lemma 6 $X(D_n; \{s_1, s_2\}) \in \mathcal{U}$ since (see, e.g., [BEFS95]),

$$X(D_n, \{s_1, s_2\}) \cong \overrightarrow{L}X(\mathbb{Z}_n, \{1, n-1\})$$

Definition 10 (Digraph $P(n,k)$, [F84]) *Given integers k and n, $1 \le k \le n-1$, $P(n,k)$ is the digraph whose vertices are the permutations on k-tuples from the set $\{1, 2, ..., n\}$ and whose arcs are of the form $((i_1\ i_2\ \ldots\ i_k), (i_2\ i_3\ \ldots\ i_k i))$, where $i \neq i_1, i_2, ..., i_k$.*

Let S_n be a symmetric group on a set $\{1, 2, ..., n\}$.

Example 11 *Let $S_n = \langle s_1, s_2 \rangle$, where $s_1 = (1\ 2\ \ldots\ n)$ and $s_2 = (1\ 2\ \ldots\ n-1)$. This is because (see, e.g., [CM72], §1.7) $S_n = \langle (1\ 2\ \ldots\ n), (1\ n) \rangle$ and $(1\ n) = (1\ 2\ \ldots\ n-1) \cdot (1\ 2\ \ldots\ n)^{-1}$. By Lemma 6 and since ([BFF97], Lemma 2.1) $X(S_n; \{s_1, s_2\}) \cong \overrightarrow{L}P(n, n-2)$, we have $X(S_n; \{s_1, s_2\}) \in \mathcal{U}$.*

Example 12 *The Cayley digraph $X(S_n;T)$, where $T = (1\ 2)\,C_{n-1}$, is the digraph of a unitary matrix. Consider $S_n = \langle S = \{(1\ 2), (1\ 2\ \ldots\ n)\} \rangle$, Then $S^{-1} = \{(1\ 2), (1\ n\ \ldots\ 2)\}$. Write $x = (1\ 2) \in S^{-1}$. Then*

$$(1\ 2)\,S = \{e, (2\ 3\ \ldots\ n)\}.$$

Consider $C_{n-1} = \langle e, (2\ 3\ \ldots\ n) \rangle$. Write

$$T = (1\ 2)\,C_{n-1} = \{(1\ 2), (1\ 2)(2\ 3\ \ldots\ n) = (1\ 2\ \ldots\ n), \ldots\}.$$

Since $S \subset T$, $S_n = \langle T \rangle$. Moreover $x \in T^{-1}$, $C_{n-1} = xT$ and $|T| = n-1 = C_{n-1}$. Then, by Lemma 6 and Lemma 8, $X(S_n;T) \in \mathcal{U}$.

2.3 Cayley digraphs of abelian groups

2.3.1 General properties

Let $conv\{P_1, ..., P_m\}$ be the convex hull of the matrices $P_1, ..., P_m \in \Pi_n$. Note that all the matrices that belong this convex hull have the same digraph. A *doubly-stochastic* matrix is a non-negative matrix whose row sums and column sums give one. The Birkhoff theorem for doubly-stochastic matrices (see, *e.g.*, [B97]) says that the set of $n \times n$ doubly-stochastic matrices is the convex hull of permutation matrices. A doubly-stochastic matrix M is *uni-stochastic* if $M_{i,j} = |U_{i,j}|^2$. The existence of a "Birkhoff-type" theorem for uni-stochastic matrices is an open problem (see, *e.g.*, [F88] and [L97]).

Let $P_1, ..., P_m$, such that $conv\{P_1, ..., P_m\} \subset \mathcal{O}$, where $\mathcal{O}$ denotes the set of uni-stochastic matrices. If a digraph D supports a uni-stochastic matrix then D supports a unitary matrix, and *viceversa*. If D supports $conv\{P_1, ..., P_m\} \subset \mathcal{O}$ then, obviously, D supports a unitary matrix. In such a case, with an abuse of notation, we write $D \in \mathcal{O}$.

Theorem 13 (Au-Young and Cheng, [AC91]) *Let $P_1, ..., P_m \in \Pi_n$. If*

$$conv\{P_1, ..., P_m\} \subset \mathcal{O}$$

then $P_1, ..., P_m$ are pairwise complementary.

Proposition 14 *If $X(G; S) \in \mathcal{O}$ then:*

1. *For every $s, t \in S$, and $1 \leq h, i, j, k \leq |G|$, if $g_j = sg_i, g_k = sg_h$ and $g_k = tg_i$ then $g_j = tg_h$.*

2. *For every $s, t \in S$, $st^{-1} = ts^{-1}$.*

3. *The order of G is even.*

4. *If G is abelian then, for every $s, t \in S$, $2s = 2t$.*

Proof. In the order:

1. By Theorem 13.

2. From 1, since $s^{-1}g_j = g_i$ and $t^{-1}g_k = g_i$, we have $s^{-1}g_j = t^{-1}g_k$, and, since $s^{-1}g_k = g_h$ and $t^{-1}g_j = g_h$, we have $s^{-1}g_k = t^{-1}g_h$. Then, since $g_k = st^{-1}g_j$, we obtain $s^{-1}g_j = t^{-1}st^{-1}g_j$ and $ts^{-1}g_j = st^{-1}g_j$, that implies $st^{-1} = ts^{-1}$. Since $st^{-1} = ts^{-1} = (st^{-1})^{-1}$, st^{-1} is an involution.

3. From point 2, since a group of odd order is without involutions.

4. From point 2, since G abelian, given that $s = ts^{-1}t = s^{-1}2t$, we have $2s = 2t$.

■

2.3.2 Cayley digraphs of cyclic groups

Proposition 15 *If $X(\mathbb{Z}_n; S) \in \mathcal{O}$ then:*

1. *$|S| = 2$ and $t = s + \frac{n}{2} \pmod n$.*
2. *$\mathbb{Z}_n = \langle s,t \rangle$ if and only if s odd, or s even and $n = 4m+2$ (that is $\frac{n}{2}$ is odd) where m is a non-negative integer.*
3. *If $\mathbb{Z}_n = \langle s,t \rangle$ then $X(\mathbb{Z}_n; \{s,t\})$ is hamiltonian.*
4. *$X(\mathbb{Z}_n; \{s,t\})$ is a graph if and only if $s = \frac{n}{4}$.*
5. *If $X(\mathbb{Z}_n; \{s,t\})$ is a graph and $\mathbb{Z}_n = \langle s,t \rangle$ then it is not hamiltonian.*
6. *$|N^+(s) \cap N^+(t)| = |N^-(s) \cap N^-(t)| = 2$.*

Proof. In the order:

1. From 4 of Proposition 14, $2s = 2t$. Let $t > s$. Then $t = s + x \pmod n$ and $2s + 2x \pmod n = 2t \pmod n$. This occurs if and only if $x = \frac{n}{2}$. Then $t = s + \frac{n}{2} \pmod n$.
2. If s and t are both even then they generate the even subgroup of order $n/2$. In the other cases, s and t generate $\mathbb{Z}_n$. Clearly if s even then t odd if and only if $n/2$ is odd, that is $n = 4m+2$.
3. From point 2, either s or t has to be odd. Since n is even, an odd element of $\mathbb{Z}_n$ has order n. Suppose s odd. In $X(\mathbb{Z}_n; \{s,t\})$ there is then an hamiltonian cycle $e, s, 2s, ..., (n-1)s, e$.
4. From point 1, $t = s + \frac{n}{2} \pmod n$. If $X(\mathbb{Z}_n; \{s,t\})$ is a graph then $t = s^{-1}$, that is $t = n - s \pmod n$. So, $n - s \pmod n = s + \frac{n}{2} \pmod n$, which implies $s = \frac{n}{4}$. The sufficiency is clear.
5. From the previous point, $X(\mathbb{Z}_n; \{s,t\})$ is a graph if and only if $s = \frac{n}{4}$. Then $n = 4m$. From 3, since s is even, we need t odd to generated $\mathbb{Z}_n$. From 2, t is odd if $n = 4m+2$. A contradiction.

■

The *distance* from a vertex v_i to a vertex v_j is denoted by $d(v_i, v_j)$ and it is the length (the number of arcs) of the shortest dipath from v_i to v_j. The *diameter* of $D = (V, A)$ is $dia(D) = \max_{(v_i,v_j) \in V \times V} d(v_i, v_j)$.

Proposition 16 *If $X(\mathbb{Z}_n; \{s,t\}) \in \mathcal{O}$ then:*

1. *It is a line digraph of the multidigraph with adjacency matrix $M = 2 \cdot M(X(\mathbb{Z}_{n/2}; \{1\}))$.*
2. *$dia(X(\mathbb{Z}_n; \{s,t\})) = \frac{n}{2} + 1$.*

Proof. In the order:

1. From 6 of Proposition 15, follows that the rows and columns of $M(D)$ are identical or orthogonal. By the Richard characterization (cfr. proof of Lemma 6), this is sufficient for a digraph to be a line digraph. Observe that the base digraph of $X(\mathbb{Z}_n;\{s,t\})$ is the multidigraph with adjacency matrix M.

2. Since $dia\left(X\left(\mathbb{Z}_{n/2};\{1\}\right)\right) = n/2$ and since the diameter of the line digraph increases of one unit in respect to the diameter of its base digraph (see, *e.g.*, [P96]), the proposition follows.

■

Remark 17 *Let $D = X(\mathbb{Z}_n;\{s,t\}) \in \mathcal{O}$. From Proposition 16, follows that the eigenvalues of D are the $n/2$ eigenvalues of the multidigraph, which are $\{2\omega^j : 0 \leq j < n/2, \omega = e^{4i\frac{\pi}{n}}\}$, plus an eigenvalue zero with multiplicity $n/2$.*

An *automorphism* of a digraph D is a permutation π of $V(D)$, such that $(v_i,v_j) \in A(D)$ if and only if $(\pi(v_i),\pi(v_j)) \in A(D)$. Let $Aut(D)$ be the group of the automorphisms of a digraph D. It is well-known that if $D = X(G;S)$ is a Cayley digraph then $Aut(D)$ contains the regular representation of G. This implies that a Cayley digraph is *vertex-transitive*, that is its automorphism group acts transitively on its vertex-set. A digraph D is *arc-transitive* if, for any pair of arcs (v_i,v_j) and (v_k,v_l), there exists a permutation $\pi \in Aut(D)$ such that $\pi(v_i) = v_k$ and $\pi(v_j) = v_l$.

Proposition 18 *If $X(\mathbb{Z}_n;\{s,t\}) \in \mathcal{O}$ then it is arc-transitive.*

Proof. Let $D = X(\mathbb{Z}_n;\{s,t\})$. Since D is a Cayley digraph, $Aut(D)$ contains the regular representation of D. Take the element $\frac{n}{2}$ and look at $\frac{n}{2}$ has an automorphism of D. The action of $\frac{n}{2}$ on s gives $s+\frac{n}{2} \pmod{n}$. The action of $\frac{n}{2}$ on $s+\frac{n}{2} \pmod{n}$ gives s. The proposition follows easily, $\frac{n}{2}(S) = S$, and $\frac{n}{2}$ can be seen as a group homomorphism. ■

Remark 19 *Consider a nearest neighbor random walk on $X(\mathbb{Z}_n;\{s,t\}) \in \mathcal{O}$, with probability $p(s) = \frac{1}{2} = q(t)$. This random walk is non-ergodic since $\gcd(t-s,n) = \frac{n}{2}$. Observe that, in Cesaro-mean, the random walk is ergodic and converges in $n/2$ steps towards uniformity. It would be interesting to observe if random walks on digraphs of unitary matrices have a characteristic behaviour.*

2.3.3 General abelian groups

Let $G = \mathbb{Z}_{p_1} \times \mathbb{Z}_{p_2} \times \cdots \times \mathbb{Z}_l$ be an abelian group written in its prime-power canonical form. An element of G has then the form $(g_1,g_2,...,g_l)$. Let

$$S = \{(s_{1_1},s_{2_1},...,s_{l_1}),(s_{1_2},s_{2_2},...,s_{l_2}),...,(s_{1_k},s_{2_k},...,s_{l_k})\}$$

be a set of generators of G. If $X(G;S) \in \mathcal{O}$ then, from 4 of Proposition 14, $2s = 2t$, for every $s,t \in S$. Then, for every i and j,

$$2(s_{1_i}, s_{2_i}, ..., s_{l_i}) = 2(s_{1_j}, s_{2_j}, ..., s_{l_j}) =$$
$$(2s_{1_i}, 2s_{2_i}, ..., 2s_{l_i}) = (2s_{1_j}, 2s_{2_j}, ..., 2s_{l_j}).$$

Proposition 20 *Let G be abelian and let $X(G;S) \in \mathcal{O}$.*

1. *If p_i is odd then $s_{i_j} = s_{i_k}$, for every j and k.*
2. *If every p_i is odd then $|S| = 1$.*

Proof. In the order:

1. Suppose that p_i is odd. From 4 of Proposition 14, $2s_{i_j} = 2s_{i_k}$. The result follows. This implies that, if $G = \langle S \rangle$ then $s_{i_j} \neq e$. In fact, if $s_{i_j} = e$ then, for every k, $s_{i_k} = e$, and, in such a case, $G \neq \langle S \rangle$.
2. It is a consequence of the previous point.

■

2.3.4 An example: the n-cube

An *n-cube* (or, equivalently, *n-dimensional hypercube*), denoted by Q_n, is a graph whose vertices are the vectors of the n-dimensional vector space over the field $GF(2)$. There is an edge between two vertices of the n-cube whenever their Hamming distance is exactly 1, where the *Hamming distance* between two vectors is the number of coordinates in which they differ. The n-cube is widely used as architecture for interconnection networks (see, *e.g.*, [H97]). The n-cube is the Cayley digraph of the group $\mathbb{Z}_2^n$, generated by the set $S = \{(1,0,...,0), (0,1,0,...,0), ..., (0,...,0,1)\}$. Since, for every $s,t \in S$, $2s = 2t$, we have $X(\mathbb{Z}_2^n; S) \in \mathcal{O}$. We observe this explicitly. Label the vertices of Q_n with the binary numbers representing $0, 1, ..., 2^n - 1$. Consider

$$M(Q_2)) = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$

A *weighing matrix of size n and weight k*, denoted by $W(k,n)$, is a $(-1,0,1)$-matrix such that $W(k,n) \cdot W(k,n)^{\intercal} = kI_n$. Clearly, $\frac{1}{\sqrt{k}}W(k,n)$ is unitary. The matrix

$$M = \begin{bmatrix} 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

is a symmetric weighing matrix, $W(2,4)$. In fact, $M = M^{\intercal}$ and $MM^{\intercal} = 2I_4$. Then $M(Q_2)$ supports a unitary matrix. The graph Q_n is constructed of two copies of Q_{n-1}, where the corresponding vertices of each subgraph are connected. The base of the construction is the graph with one vertex. The matrix

$$W(3,8) = \begin{bmatrix} W(2,4) & -I_4 \\ I_4 & W(2,4) \end{bmatrix}$$

is supported by Q_3 and is again a weighing matrix, since $W(2,4)$ is symmetric. Note that $W(3,8)$ is not symmetric. So, in general,

$$W\left(k,2^k\right) = \begin{bmatrix} W\left(k-1,2^{k-1}\right) & -I_{2^{k-1}} \\ I_{2^{k-1}} & W\left(k-1,2^{k-1}\right)^{\intercal} \end{bmatrix},$$

is a weighing matrix supported by Q_n. Note that if A is an $n \times n$ unitary matrix then the block-matrix

$$\begin{bmatrix} A & -I_n \\ I_n & A^{\intercal} \end{bmatrix}$$

is unitary under renormalization, since

$$\begin{bmatrix} A & -I_n \\ I_n & A^{\intercal} \end{bmatrix} \cdot \begin{bmatrix} A^{\intercal} & I_n \\ -I_n & A \end{bmatrix} = \begin{bmatrix} 2I_n & 0 \\ 0 & 2I_n \end{bmatrix}$$

Remark 21 *The graph obtained by adding a self-loop at each vertex of the n-cube also supports a unitary matrix. The unitary matrix*

$$\frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & -1 & 0 \\ 1 & -1 & 0 & 1 \\ -1 & 0 & -1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}$$

can be seen as the building-block of the iteration.

Remark 22 *Let D be a Cayley digraph. If $D \in \mathcal{U}$ then D is not necessarily a line digraph. The n-cube is a counter-example. In fact, $Q_n \in \mathcal{U}$ and it is not a line digraph.*

Remark 23 *Let D be the digraph on n vertices, and let $D \in \mathcal{U}$. Let U be a unitary matrix supported by D. If the order of $U \in U(n)$ is k then U generates a cyclic group $\{U, U^2, ..., U^k = I_n\} \subset U(n)$. It would be interesting to study if the digraphs of the matrices $U, U^2, ..., U^{k-1}$ have some common properties, apart from, trivially, the same number of vertices.*

3 Digraphs in general

3.1 Proof of Theorem 2

Proof of Theorem 2. Suppose that $(v_i, v_j) \in A(D)$ is a directed bridge. We can then label $V(D)$ such that $M(D)$ has the form

$$\begin{bmatrix} & M_1 & & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} & & \mathbf{0} & \\ M_{i,1} & \cdots & M_{i,i} & 1 & 0 & \cdots & 0 \\ & \mathbf{0} & & \begin{matrix} M_{i+1,j} \\ \vdots \\ M_{n,j} \end{matrix} & & M_2 & \end{bmatrix},$$

where $M_{i,1}, ..., M_{i,i}, M_{i+1,j}, ..., M_{n,j} \in \{0,1\}$. Suppose that $D \in \mathcal{U}$. Then D is *quadrangular* (the term "quadrangular" has been coined in [GZ98]), that is, for every v_i and v_j, $|N^-(v_i) \cap N^-(v_j)| \neq 1$ and $|N^+(v_i) \cap N^+(v_j)| \neq 1$. If this condition holds then $M_{i,j}$ is the *only* non-zero entry in the i-th row and the j-th column of $M(D)$. Then the form of $M(D)$ is

$$\begin{bmatrix} M' & & \\ & 1 & \\ & & M'' \end{bmatrix},$$

where the matrix M' is $(i-1) \times i$ and the matrix M'' is $(n-i+1) \times (n-i+2)$. If $D \in \mathcal{U}$ then M' and M'' have to be square. Then $D \notin \mathcal{U}$. A contradiction.

Suppose that $\{v_i, v_j\}$ is a bridge. Then $M_{i+1,i} = 1$. A similar reasoning as in the case of directed bridges applies. This forces $M(D)$ to take one of the two forms

$$\begin{bmatrix} M' & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & M'' \end{bmatrix} \text{ and } \begin{bmatrix} M' & & & \\ & 1 & 1 & \\ & 1 & 1 & \\ & & & M'' \end{bmatrix},$$

where M' is $(i-1) \times (i-1)$ and M'' is $(n-1+2) \times (n-i+1)$. Clearly, $D \in \mathcal{U}$ if and only if M' and M'' support unitary matrices.

Suppose that v_i is a cut-vertex. We can then label $V(D)$ such that $M(D)$ has the form

$$\begin{bmatrix} & M_1 & & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} & & \mathbf{0} & \\ M_{i,1} & \cdots & M_{i,i} & M_{i,i+1} & & \cdots & M_{i,n} \\ & \mathbf{0} & \begin{matrix} M_{i+1,i} \\ \vdots \\ M_{n,i} \end{matrix} & & & M_2 & \end{bmatrix},$$

where $M_{i,1}, ..., M_{i,n}, M_{i+1,i}, ..., M_{n,i} \in \{0,1\}$, but not all are zero. Suppose that $D \in \mathcal{U}$. It is immediate to observe that a similar reasoning as in the previous cases applies again, forcing the cut-vertex to be in a connected component that is either $\overleftrightarrow{K}_2$ or $\overleftrightarrow{K}_2^+$. ■

3.2 Corollaries

Here we observe some corollaries of Theorem 3.

Corollary 24 *Let D be a connected graph on $n+2$ vertices and let $D \in \mathcal{U}$. Then D is 2-vertex-connected and 2-edge-connected.*

Corollary 25 *Let D be a connected graph on $n > 2$ vertices and let $D \in \mathcal{U}$. Then D contains at least two independent paths between any two vertices.*

Proof. From the Global Version of Menger's theorem (see, *e.g.*, [D00], Theorem 3.3.5). ■

Corollary 26 *Let D be a connected graph on $n \geq 3$ vertices and let $D \in \mathcal{U}$. Then, for all $v_i, v_j \in V(D)$, where $v_i \neq v_j$, there exists a cycle containing both v_i and v_j.*

Proof. From Theorem 3.15 in [M01]. ■

A *k-flow* in a graph D is an assignment of an orientation of D together with an integer $c \in \{1, 2, ..., k-1\}$ such that, for each vertex v_i, the sum of the values of c on the arcs into v_i equals the sum of the values of c on the arcs from v_i.

Corollary 27 *Let D be a graph. If $D \in \mathcal{U}$ then it has a 6-flow.*

Proof. From Seymour's theorem [S81]. ■

Remark 28 *A* cycle cover *of a graph D is a set of cycles, such that every edge of D lies in at least one of the cycles. The length of a cycle cover is the sum of the lengths of its cycles. If $D \in \mathcal{U}$ the it has a cycle cover with length at most $\frac{|A(D)|}{2} + \frac{25}{24}(V(D) - 1)$, since this result holds for bridgeless graphs [F97].*

Remark 29 *In a connected graph, a* pendant-vertex *is a vertex with degree 1. The graph of a unitary is without pendant-vertices. Zbigniew [Z82] proved that the probability that a random graph on n vertices has no pendant vertices goes to 1 as n goes to ∞. Is a random graph bridgeless?*

Remark 30 *A graph D is said to be* eulerian *if D is connected and the degree of every vertex is even. An eulerian graph D is said to be* even *(odd) if it has an even (odd) number of edges. Delorme and Poljak [DP93] stated the following conjecture which Steger confirmed for $d = 3$: for $d \geq 3$, every bridgeless d-regular graph D admits a collection of even eulerian subgraphs such that every edge of D belongs to the same number of subgraphs from the collection. It would be interesting to verify if the conjecture is confirmed by the graphs of unitary matrices.*

3.3 Matchings

The *term rank* of a matrix is the maximum number of nonzero entries of the matrix, such that no two of them are in the same row or column. Let $M_1 \circ M_2$ be the *Hadamard product* of matrices M_1 and M_2: $(M_1 \circ M_2)_{ij} = M_{1_{ij}} M_{2_{ij}}$.

Proposition 31 *Let D be a digraph and let $D \in \mathcal{U}$. Then there exists a permutation matrix P, such that $M(D) \circ P = P$.*

Proof. If a digraph on n vertices $D \in \mathcal{U}$ then the term rank of $M(D)$ is n. In fact, it is well-known that the possible maximum rank of a matrix with digraph D is equal to its term rank, that is the term rank of $M(D)$. The proposition follows. ■

A *cycle factor* of a digraph D is a collection of pairwise vertex-disjoint dicycles spanning D. In other words, a cycle factor is a spanning 1-regular subdigraph of D.

Proposition 32 *The digraph of a unitary matrix has at least a cycle factor*

Proof. By Proposition 31, since the adjacency matrix of a cycle factor is a permutation matrix. ■

Remark 33 *The existence of a cycle factor and strong connectdness are necessary and sufficient conditions for some families of digraphs to be hamiltonian (see,* e.g.*, [B-JG01]).*

In a graph D, a *perfect 2-matching* is a spanning subgraph consisting of vertex-disjoint edges and cycle. A perfect 2-matching is what Tutte calls *Q-factor* [T53].

Proposition 34 *Let D be a graph without loops and let $D \in \mathcal{U}$. Then D has a perfect 2-matching.*

Proof. By Proposition 31, there is a permutation matrix P such that $M(D) \circ P = P$. Since $M(D)$ is symmetric, there is P^{-1} such that $M(D) \circ P + P^{-1} = P + P^{-1}$. Clearly, P can be symmetric itself and in such a case $P \circ P^{-1} = P$. The proposition follows. We consider a graph without loops, because in such a case P might have a fixed-point, and the fact $M(D) \circ P = P$ would not necessarily implies a perfect 2-matching. ■

Proposition 35 *Let D be a graph and let $D \in \mathcal{U}$. Then, for every $S \subset V(D)$, $|S| \leq |N(S)|$.*

Proof. Let U be a unitary matrix acting on an complex vector space $\mathcal{H}$. Since U is invertible and since $U^{-1} = U^{\dagger}$, U is an isomorphism from $\mathcal{H}$ onto $\mathcal{H}$. The proposition follows, as a consequence of the fact that an isomorphism is a bijective map. ■

In a graph D on $n = 2k$ vertices, a *matching* is collection of pairwise vertex-disjoint graphs $\overleftrightarrow{K}_{2_i}$. If a matching has $n/2$ members it is then called *perfect matching.*

Proposition 36 *Let D be a bipartite graph and let $D \in \mathcal{U}$. Then D has at least a perfect matching.*

Proof. By Proposition 35, together with the König-Hall matching theorem (see, *e.g.*, [LP86]). ∎

Remark 37 *A graph D has a perfect matching if and only if there exists a symmetric permutation matrix P without fixed points, such that $M(D) \circ P = P$. The conditions for the existence of perfect matchings in non-bipartite graphs of unitary matrices remain to be studied.*

3.4 A remark: perfect 2-matchings and the Sperner capacity of a graph

We observe now a consequence of Proposition 34. Consider a probability measure μ with domain $V(D)$. Let $\{v_i, v_j\}$ be an edge of D. The vertices v_i and v_j induces a subgraph $\overleftrightarrow{K}_2$. All the subgraphs of D induced by two connected vertices form the *edge family* of D, denoted by $\mathcal{F}(D)$. The *entropy* of $\overleftrightarrow{K}_2$ (see, *e.g.*, [GKV94]) is defined by

$$H(\{v_i, v_j\}, \mu) = [\mu(v_i) + \mu(v_j)] \cdot h\left(\frac{\mu(v_i)}{\mu(v_i) - \mu(v_j)}\right),$$

where h denotes the binary entropy function

$$h(x) = -x \log_2 x - (1-x) \log_2 (1-x).$$

The *Sperner capacity* of $\mathcal{F}(D)$ [CKS88] is

$$\Theta(\mathcal{F}(D)) = \max_{\Pr} \min_{\{v_i, v_j\} \text{ in } D} H(\{v_i, v_j\}, \mu).$$

This quantity has an information theoretical interpretation (it is related to the zero-error capacity of channels) and it is used in the asymptotic solution of various problems in extremal set theory (determination of the asymptotic of the largest size of qualitative independent partitions in the sense of Rényi) [GKV94].

Proposition 38 *Let D be a graph and let $D \in \mathcal{U}$. Then $\Theta(\mathcal{F}(D)) = \frac{2}{n}$ and the corresponding probability distribution is uniform over $V(D)$.*

Proof. By Proposition 34 and by Theorem 1 in [G98]. ∎

3.5 A conjecture about hamiltonian cycles

Let $D \in \mathcal{U}$ be a connected graph on n vertices. It is licit to ask if the fact that $D \in \mathcal{U}$ is a sufficient condition for the existence of hamiltonian cycles. Take as hypothesis the quadrangularity condition and the existence of a perfect 2-matching. If $n = 2, ..., 6$, it can be shown that these two facts, together, imply the existence of an hamiltonian cycle.

Conjecture 39 *Let D be a connected graph and let $D \in \mathcal{U}$. Then D is hamiltonian.*

Remark 40 *A* claw *is the bipartite graph $K_{1,3}$. Let $\underline{\lambda}$ be the graph with adjacency matrix*

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$

We know that if D is 2-vertex-connected and if no induced subgraph of D is isomorphic to $K_{1,3}$ or to $\underline{\lambda}$, then D is hamiltonian (see, e.g., *[M01], Theorem 5.15). These conditions are not sufficient to show that if $D \in \mathcal{U}$ then D is hamiltonian. A counterexample is the graph D with adjacency matrix*

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

Since the matrix

$$\begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

is unitary, $D \in \mathcal{U}$. It is easy to see that D is hamiltonian even if D has a claw. Its adjacency matrix is

$$\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix},$$

a submatrix of $M(D)$.

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