Conjecture on Hamilton Cycles in Digraphs of Unitary Matrices

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Abstract

We conjecture new sufficient conditions for a digraph to have a Hamilton cycle. In view of applications, the conjecture is of interest in the areas where unitary matrices are of importance including quantum mechanics and quantum computing.

Keywords: digraph, Hamilton cycle, sufficient conditions, conjecture, quantum mechanics, quantum computing.

1 Introduction

For a digraph $D = (V, A)$ and $x \neq y \in V$, we say that x *dominates* y, denoted $x \rightarrow y$, if $xy \in A$. All vertices dominated by x are called the *out-neighbors* of x; we denote the set of out-neighbors by $N^+(x)$. All vertices that dominate x are *in-neighbors* of x; the set of in-neighbors is denoted by $N^-(x)$. The number of out-neighbors (in-neighbors) of x is the *out-degree* $d^+(x)$ of x (*in-degree* $d^-(x)$ of x). The maximum *semi-degree* $\Delta^0(D)$ is the least integer k such that $k \geq d^+(x)$ and $k \geq d^-(x)$ for each $x \in V$.

A set $S \subseteq V$ is called an *out-set* (*in-set*, respectively) if S has at least two vertices and, for every $u \in S$, there exists $v \in S, v \neq u$ such that $N^+(u) \cap N^+(v) \neq \emptyset$ ($N^-(u) \cap N^-(v) \neq \emptyset$, respectively). A digraph D is called *s-quadrangular* if, for every out-set S, we have $|\cup (N^+(u) \cap N^+(v) : u \neq v, u, v \in S)| \geq |S|$ and, for every in-set S, we have $|\cup (N^-(u) \cap N^-(v) : u, v \in S)| \geq |S|$.

A collection of disjoint cycles that include all vertices of D is called a *cycle factor* of D. We denote a cycle factor as the union of cycles $C_1 \cup \cdots \cup C_t$, where the cycles C_i are

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disjoint and every vertex of D belongs to a cycle C_j. If $t = 1$, we say that C_1 is a *Hamilton cycle* of D. A digraph with a Hamilton cycle is called *hamiltonian*. Clearly, the existence of a cycle factor is a necessary condition for a digraph to be hamiltonian.

A digraph D is *strong* if there is a path from x to y for every ordered pair x, y of vertices of D. Clearly, a hamiltonian digraph is strong.

A complex $n \times n$ matrix U is *unitary* if $U \cdot U^\dagger = U^\dagger \cdot U = I_n$, where $U^\dagger$ denotes the conjugate transpose of U and I_n the $n \times n$ identity matrix. The *digraph of* an $n \times n$ matrix M (over any field) is a digraph on n vertices with an arc ij if and only if the (i, j)-the entry of the M is nonzero. A matrix M (over any field) is *irreducible* if there does not exist a permutation matrix P such that PMP^{-1} is block-diagonal. It is clear that the digraph of an irreducible matrix is strong. It was shown in [9] that the digraph of a unitary matrix is s-quadrangular. S-quadrangular tournaments were studied in [7]. We believe that the following claim holds:

Conjecture 1.1 *Every strong s-quadrangular digraph has a Hamilton cycle.*

It follows that if Conjecture 1.1 is true, then the digraph of an irreducible unitary matrix is hamiltonian. In our view, the conjecture is of real interest due to the following reasons. Unitary matrices are important in quantum mechanics and, at present, are central in the theory of quantum computation [8]. In particular, we may associate a strong digraph to a quantum system whose unitary evolution allows transitions only along the arcs of the digraph (that is, respecting the topology of the graph, like in discrete quantum walks [1, 6]). Then, if the conjecture is true, the digraph would be necessarily hamiltonian. Moreover, the conjecture is important in the attempt to understand the combinatorics of unitary and unistochastic matrices, see, e.g., [3, 4, 11]. Finally, there are several sufficient conditions for hamiltonicity of directed and undirected graphs (see, e.g., [2, 5]). Our conjecture appears to be an interesting, natural and difficult addition to the list of open problems in the area.

In this paper, we provide some support to the conjecture. In Section 2, we show that if a strong s-quadrangular digraph D has the maximum semi-degree at most 3, then D is hamiltonian. In our experience, to improve the result by replacing $\Delta^0(D) \leq 3$ with $\Delta^0(D) \leq 4$ appears to be a very difficult task. In Section 3 we managed to show the improved result only for the case of undirected graphs. Even in this special case the proof is fairly non-trivial.

The number of neighbors of a vertex x of an undirected graph G is called the *degree* of x and denoted by $d(x)$. The *complete biorientation* of an undirected graph G is a digraph obtained from G by replacing every edge xy by the pair xy, yx of arcs. A graph is *s-quadrangular* if its complete biorientation is s-quadrangular.

2 Supporting Conjecture 1.1 for s-quadrangular digraphs

The existence of a cycle factor is a natural necessary condition for a digraph to be hamiltonian. The following assertion verifies this condition for strong s-quadrangular digraphs.

Theorem 2.1 *Every strong s-quadrangular digraph $D = (V, A)$ has a cycle factor.*

Proof: By Proposition 3.11.6 in [2], a digraph H has a cycle factor if and only if, for every $X \subseteq V(H)$, $|\cup_{x\in X} N^+(x)| \geq |X|$ and $|\cup_{x\in X} N^-(x)| \geq |X|$.

Let $X \subseteq V$. If X is an out-set, then

$$|X| \leq |\cup (N^+(u) \cap N^+(v) : u \neq v, u, v \in X)| \leq |\cup_{x\in X} N^+(x)|.$$

If X is not an out-set, then consider a maximal subset S of X, which is an out-set. Since D is strong every vertex of X dominates a vertex. Moreover, since every vertex of $X - S$ dominates a vertex that is not dominated by another vertex in X, we have $|\cup_{x\in X-S} N^+(x)| \geq |X - S|$. Thus,

$$|\cup_{x\in X} N^+(x)| \geq |X - S| + |\cup_{x\in S} N^+(x)| \geq |X - S| + |S| = |X|.$$

Similarly, we can show that $|\cup_{x\in X} N^-(x)| \geq |X|$ for each $X \subseteq V$. □

Now we are ready to prove the main result of this section.

Theorem 2.2 *If the out-degree and in-degree of a vertex in a strong s-quadrangular digraph D are at most 3, then D is hamiltonian.*

Proof: Suppose that $D = (V, A)$ is a non-hamiltonian strong s-quadrangular digraph and for every vertex $u \in V$, $d^+(u), d^-(u) \leq 3$.

Let $F = C_1 \cup \cdots \cup C_t$ be a cycle factor of D with minimum number $t \geq 2$ of cycles. Assume there is no cycle factor $C'_1 \cup \cdots \cup C'_t$ such that $|V(C'_1)| < |V(C_1)|$. For a vertex u on C_i we denote by u^+ (u^-) the successor (the predecessor) of u on C_i. Also, $x^{++} = (x^+)^+$. Since every vertex belongs to exactly one cycle of F these notation define unique vertices. Let u, v be vertices of C_i and C_j, $i \neq j$, respectively and let $K(u, v) = \{uv^+, vu^+\}$. At least one of the arcs in $K(u, v)$ is not in D as otherwise we may replace the pair C_i, C_j of cycles in F with just one cycle $uv^+v^{++} \ldots vu^+u^{++} \ldots u$, a contradiction to minimality of t.

Since D is strong, there is a vertex x on C_1 that dominates a vertex y outside C_1. Without loss of generality, we may assume that y is on C_2. Clearly, $\{x, y^-\}$ is an out-set. Since $K(x, y^-) \not\subset A$ and $x \rightarrow y$, we have $y^- \not\rightarrow x^+$. This is impossible unless $d^+(x) > 2$. So, $d^+(x) = 3$ and there is a vertex $z \notin \{x^+, y\}$ dominated by both x and y^-. Let z be on C_j.

Suppose that $j \neq 1$. Since $K(x, z^-) \not\subset A$ and $x \rightarrow z$, we have $z^- \not\rightarrow x^+$. Since $\{x, z^-\}$ is an out-set, we have $z^- \rightarrow y$. Suppose that $j \geq 3$. Since $z^- \rightarrow y$ and $y^- \rightarrow z$, we have $K(y^-, z^-) \subset A$, which is impossible. So, $j = 2$. Observe that $\{x^+, z\}$ is an in-set ($x \rightarrow x^+$ and $x \rightarrow z$). But $y^- \not\rightarrow x^+$ and $z^- \not\rightarrow x^+$. Hence, $|N^-(x^+) \cap N^-(z)| = 1$, which is impossible.

Thus, $j = 1$. Since $K(y^-, z^-) \not\subset A$ and $y^- \rightarrow z$, we have $z^- \not\rightarrow y$. Since $\{x, z^-\}$ is an out-set, $z^- \rightarrow x^+$. By replacing C_1 and C_2 in F with $x^+x^{++} \dots z^-x^+$ and $xyy^+ \dots y^-zz^+ \dots x$ we get a cycle factor of D, in which the first cycle is shorter than C_1. This is impossible by the choice of F. □

3 Supporting Conjecture 1.1 for undirected s-quadrangular graphs

Let $e(X, Y)$ denote the number of edges with one endpoint in X and one endpoint in Y. We write $e(X) = e(X, X)$ to denote the number of edges in $G\langle X \rangle$. The following lemma is of interest for arbitrary undirected graphs. To the best of our knowledge, no claim of this lemma was published before.

Lemma 3.1 *If $G = (V, E)$ is a graph with no cycle factor, then we can partition $V(G)$ into S, T, O and R, such that the following properties hold.*

(i): *T is independent.*

(ii): *$e(R, O \cup T) = 0$.*

(iii): *Every connected component in $G\langle O \rangle$ has an odd number of edges into T.*

(iv): *No $t \in T$ has two edges into the same connected component of $G\langle O \rangle$.*

(v): *For every vertex $o \in O$ we have $e(o, T) \leq 1$.*

(vi): *There is no edge $ot \in E(G)$, where $t \in T$, $o \in O$, such that $e(t, S) = 0$ and $e(o, O) = 0$.*

(vii): *$|T| - |S| - \frac{e(T,O) - oc(S,T)}{2} > 0$, where $oc(S, T)$ is the number of connected components in $G - S - T$, which have an odd number of edges into T. (Note that $oc(S, T)$ is also the number of connected components of $G\langle O \rangle$, by (ii) and (iii).)*

Proof: Let G be an arbitrary graph with no cycle factor. Observe that if some vertex $x \in V(G)$ has degree zero, then the lemma holds with $O = S = \emptyset$, $T = \{x\}$ and $R = V - \{x\}$. Similarly if some vertex $x \in V(G)$ has degree one, where $N(x) = \{y\}$, then the lemma holds with $S = \emptyset$, $T = \{x\}$ and O consisting of the vertices of the connected

component in $G\langle V-\{x\}\rangle$, which contains y. In this case $R = V - T - O$. Therefore we may assume that the minimum degree of a vertex in G is two.

By Tutte's f-factor Theorem (see Exercise 3.3.16 in [10]), there exists disjoint subsets S and T of V, such that the following holds.

$$oc(S,T) + 2|T| - \sum_{v \in T} d_{G-S}(v) > 2|S|$$

Thus,

$$w(S,T) = |T| - |S| - e(T) - \frac{e(T, V-S-T) - oc(S,T)}{2} > 0$$

We now choose disjoint subsets S and T of V, such that the following holds in the order it is stated.

- maximize $w(S,T)$
- minimize $|T|$
- maximize $|S|$
- minimize $oc(S,T)$

Furthermore, let O contain all vertices in $V-S-T$ belonging to connected components of $G\langle V-S-T\rangle$, each of which has an odd number of edges into T. Let $R = V-S-T-O$. We will prove that S, T, O and R satisfy (i)-(vii).

Clearly, $w(S,T) > 0$. Let $t \in T$ be arbitrary and assume that t has edges into i connected components in $G\langle O\rangle$. Let $S' = S$ and let $T' = T - \{t\}$. Furthermore let $j = 1$ if the connected component in $G\langle V - S' - T'\rangle$ containing t has an odd number of edges into T', and $j = 0$, otherwise. Observe that $|T'| = |T| - 1$, $e(T') = e(T) - e(t,T)$, $e(T', V-S'-T') = e(T, V-S-T) - e(t, V-S-T) + e(t,T)$ and $oc(S',T') = oc(S,T) - i + j$. Since $|T'| < |T|$, we must have $w' = w(S',T') - w(S,T) < 0$. Therefore, we have

$$w' = -1 + e(t,T) + \frac{e(t, V-S-T) - e(t,T) - i + j}{2} < 0.$$

Thus,

$$e(t,T) + e(t, V-S-T) - i + j \leq 1 \tag{1}$$

Observe that, by the definition of i, $e(t, V-S-T) \geq i$. Now, by (1), $i \leq e(t, V-S-T) \leq i - j - e(t,T) + 1$. Thus, $j + e(t,T) \leq 1$ and, if $e(t,T) > 0$, then $e(t,T) = 1$, $j = 0$ and $e(t, V-S-T) = i$. However, $e(t,T) = 1$, $e(t, V-S-T) = i$ and a simple parity argument imply $j = 1$, a contradiction.

So $e(t,T)=0$. In this case, $e(t,V-S-T)-i=0$ or 1. If $e(t,V-S-T)-i=1$, then, by a simple parity argument, we get $j=1$, which is a contradiction against (1). Therefore, we must have $e(t,V-S-T)=i$.

It follows from $e(t,T)=0$, $e(t,V-S-T)=i$, $w(S,T)>0$ and the definition of O that (i), (ii), (iii), (iv) and (vii) hold. We will now prove that (v) and (vi) also hold. Suppose that there is a vertex $o\in O$ with $e(o,T)>1$. Let $S'=S\cup\{o\}$ and $T'=T$, and observe that

$$w(S',T')-w(S,T)=-1+(e(o,T)-(oc(S,T)-oc(S',T'))/2<0 \qquad (2)$$

If $e(o,T)\geq 3$ then, by (2), $oc(S,T)>oc(S',T')+1$. However, by taking o from O, we may decrease $oc(S,T)$ by at most 1, a contradiction. So, $e(o,T)=2$ and, by (2), $oc(S,T)>oc(S',T')$. However, since $e(o,T)$ is even, taking o from O will not decrease $o(S,T)$, a contradiction. Therefore (v) holds.

Suppose that there is an edge $ot\in E(G)$, where $t\in T$, $o\in O$, such that $e(t,S)=0$ and $e(o,O)=0$. Let $S'=S$ and $T'=T\cup\{o\}-\{t\}$. By (iii) and (iv), the connected component in $G\langle V-S'-T'\rangle$, which contains t, has an odd number of arcs into T'. This implies that $oc(S',T')-oc(S,T)=-e(t,O)+1$. Also, $e(T,V-S-T)=e(T',V-S'-T')+e(t,O)-1$. By (v) we have $e(T')=0$. The above equalities imply that $w(S',T')=w(S,T)$. Since the degree of t is at least 2 and $e(t,S)=0$, we conclude that $e(t,O)\geq 2$. Thus, $oc(S',T')<oc(S,T)$, which is a contradiction against the minimality of $oc(S,T)$. This completes that proof of (vi) and that of the lemma. □

A cycle factor of an undirected graph contains no cycle of length 2. Thus, the following theorem cannot be deduced from Theorem 2.1.

Theorem 3.2 *Every s-quadrangular graph contains a cycle factor.*

Proof: Suppose G is a s-quadrangular graph with no cycle factor. Let S, T, O and R be defined as in Lemma 3.1. First suppose that there exists a vertex $t\in T$ with $e(t,S)=0$. Let $y\in N(t)$ be arbitrary, and observe that $y\in O$, by (i) and (ii). Furthermore observe that $e(y,O)\geq 1$ by (vi), and let $z\in N(y)\cap O$ be arbitrary. Since $y\in N(t)\cap N(z)$, there must exist a vertex $u\in N(t)\cap N(z)-\{y\}$, by the definition of a s-quadrangular graph. However, $u\notin O$ by (iv) and $u\notin R$ by (ii) and $u\notin T$ by (i) and $u\notin S$ as $e(t,S)=0$. This contradiction implies that $e(t,S)>0$ for all $t\in T$.

Let $S_1=\{s\in S:\ e(s,T)\leq 1\}$ and let $W=T\cap N(S-S_1)$. Observe that for every $w\in W$ there exists a vertex $s\in S-S_1$, such that $w\in N(s)$. Furthermore, there exists a vertex $w'\in T\cap N(s)-\{w\}$, by the definition of S_1. Note that $w'\in W$, which proves that for every $w\in W$, there is another vertex, $w'\in W$, such that $N(w)\cap N(w')\neq\emptyset$. Let $Z=\cup(N(u)\cap N(v):\ u\neq v\in W)$. By (i), (ii) and (v), $Z\subseteq S-S_1$. By (iii), $oc(S,T)\leq e(T,O)$ and, thus, by (vii), $|S|<|T|$. Observe that $|N(S_1)|\leq|S_1|$. The last two inequalities and the fact that $e(t,S)>0$ for all $t\in T$ imply $|Z|\leq|S-S_1|<|T-N(S_1)|\leq|W|$. This is a contradiction to the definition of a s-quadrangular graph. □

The next theorem is the main result of this section.

Theorem 3.3 *If the degree of every vertex in a connected s-quadrangular graph G is at most 4, then G is hamiltonian.*

Proof: Suppose that $G = (V, E)$ is not hamiltonian. Let $C_1 \cup C_2 \cup \cdots \cup C_m$ be a cycle factor with the minimum number $m \geq 2$. Notice that each cycle C_i is of length at least three.

For a vertex v on C_i, v^+ is the set of the two neighbors of v on C_i. We will denote the neighbors by v_1 and v_2. The following simple observation is of importance in the rest of the proof:

$$\text{If } u, v \text{ are vertices of } C_i, C_j,\ i \neq j, \text{ respectively, and } uv \in E, \text{ then } e(u^+, v^+) = 0.$$

Indeed, if $e(u^+, v^+) > 0$, then by deleting one edge from each of C_i, C_j and adding an edge between u^+ and v^+ and the edge uv, we may replace C_i, C_j by just one cycle, which contradicts minimality of m.

We prove that every vertex u which has a neighbor outside its cycle C_i has degree 4. Suppose $d(u) = 3$. Let $uv \in E$ such that $v \in C_j$, $j \neq i$. Since u, v_1 must have a common neighbor $z \neq v$, we conclude that $e(u^+, v^+) > 0$, which is impossible.

Since G is connected, there is a vertex $u \in C_1$ that has a neighbor outside C_1. We know that $d(u) = 4$. Apart from the two vertices in u^+, the vertex u is adjacent to two other vertices x, y. Assume that x, y belong to C_i, C_j, respectively. Moreover, without loss of generality, assume that $i \neq 1$. Since x_k $(k = 1, 2)$ and u have a common neighbor different from x, u_1 and u_2, we conclude that y is adjacent to both x_1 and x_2. Since $d(y) < 5$, we have $|\{u, x_1, x_2, y_1, y_2\}| < 5$. Since u, x_1, x_2 are distinct vertices, without loss of generality, we may assume that y_2 coincides with either x_1 or u. If $y_2 = u$, then $y \in u^+$ and x_1 is adjacent to a vertex in u^+, which is impossible.

Thus, $y_2 = x_1$. This means that the vertices $y_1, y, x_1 = y_2, x, x_2$ are consecutive vertices of C_i. Recall that $x_2 y \in E$. Suppose that C_i has at least five vertices. Then $y_1, y_2 = x_1, x_2$ and u are all distinct neighbors of y. Since u_1 and y have a common neighbor different from u, the vertex u_1 is adjacent to either y_1 or y_2 or x_2, each possibility implying that $e(u^+, x^+) + e(u^+, y^+) > 0$, which is impossible.

Thus, C_i has at most four vertices. Suppose C_i has tree vertices: x, y, x_1. Since u and y must have a common neighbor different from x, $y \in x^+$ is adjacent to a vertex in u^+, which is impossible. Thus, C_i has exactly four vertices: y, $x_1 = y_2$, x and $x_2 = y_1$. The properties of u and C_i that we have established above can be formulated as the following general result:

Claim A: *If a vertex w belonging to a cycle C_p is adjacent to a vertex outside C_p, then w is adjacent to a pair w' and w'' of vertices belonging to a cycle C_q of length four,*

$q \neq p$, such that w' and w'' are not adjacent on C_q.

By Claim A, x and y are adjacent not only to u, but also to another vertex $v \notin \{u, u_1, u_2\}$ of C_1, and C_1 is of length four.

For the vertex set $S = \{u, x_1, x_2\}$ there must be a set T with at least three vertices such that each $t \in T$ is a common neighbor of a pair of vertices in S. This implies that there must be a vertex $z \notin \{x, y, u_1, u_2, u, v\}$ adjacent to both x_1 and x_2. Thus, z is on C_k with $k \notin \{1, i\}$. By Claim A, x_1 and x_2 are also adjacent to a vertex s on C_k different from z_1 and z_2. Continue our argument with z_1 and z_2 and similar pairs of vertices, we will encounter cycles $Z_1, Z_2, Z_3, \ldots$ ($Z_j = z_j^1 z_j^2 z_j^3 z_j^4 z_j^1$) such that $\{z_j^2 z_{j+1}^1, z_j^4 z_{j+1}^1, z_j^2 z_{j+1}^3, z_j^4 z_{j+1}^3\} \subset E$ for $j = 1, 2, 3, \ldots$. Here $Z_1 = C_1, Z_2 = C_i, Z_3 = C_k$.

Since the number of vertices in G is finite, after a while we will encounter a cycle Z_r that we have encountered earlier. We have $Z_r = Z_1$ since for each $m > 1$ after we encountered Z_{m+1} we have established all neighbors of the vertices in Z_m. This implies that $z_1^1 z_1^2 z_1^3 z_1^4 z_2^1 z_2^2 z_2^3 z_2^4 \ldots z_{r-1}^1 z_{r-1}^2 z_{r-1}^3 z_{r-1}^4 z_1^1$ is a cycle of G consisting of the vertices of the cycles $Z_1, Z_2, \ldots, Z_{r-1}$. This contradicts minimality of m. □

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