

GRAPH INVERTIBILITY

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ABSTRACT. Extending the work of Godsil and others, we investigate the notion of the inverse of a graph (specifically, of bipartite graphs with a unique perfect matching). We provide a concise necessary and sufficient condition for the invertibility of such graphs and generalize the notion of invertibility to multigraphs. We examine the question of whether there exists a “litmus subgraph” whose bipartiteness determines invertibility. As an application of our invertibility criteria, we quickly describe all invertible unicyclic graphs. Finally, we describe a general combinatorial procedure for iteratively constructing invertible graphs, giving rise to large new families of such graphs.

1. INTRO

Given the plethora of composition operations on graphs¹ (Cartesian sum, tensor product, etc.), one is naturally led to the question of whether or not there is a sensible notion of the *inverse* of a graph. There is no shortage of possible definitions: A first attempt is to define two graphs to be inverses if they possess inverse adjacency matrices. This turns out to be overly restrictive, as under this definition only the graphs nK_2 are invertible, with themselves as their own inverses ([5]). A second attempt, motivated by the observation that the eigenvalues of the sum and product of two graphs are the pairwise sums and products of the eigenvalues of the original graphs, is to call a graph G invertible if there exists another graph G^{-1} such that for each eigenvalue λ of G , $\frac{1}{\lambda}$ is an eigenvalue of G^{-1} (with the same multiplicity). This definition too allows some unfortunate phenomena: If G_1 and G_2 are cospectral and non-isomorphic, then G_1^{-1} and G_2^{-1} (if such graphs exist) both satisfy the criterion for being inverses to G_1 , and we are left with multiple non-isomorphic inverses. Further, there would be no hope of attaining the obviously desirable property that $(G^{-1})^{-1}$ be isomorphic to G .

It therefore behooves us to strengthen the condition defining the inverse. We begin by noting that since adjacency matrices are diagonalizable (being real and symmetric), two such matrices are cospectral if and only if they are similar. The reciprocal eigenvalue condition described above is thus tantamount to asserting that the inverse A^{-1} of the adjacency matrix to G is similar to the adjacency matrix of G^{-1} . A strengthening of the definition comes from a result of Godsil ([4]) that under certain conditions on G (described below), the inverse adjacency matrix A^{-1} is in fact *signable* to a non-negative symmetric integral matrix with zeros on the diagonal, i.e., to the adjacency matrix of a graph. Here we say A is signable to B if A can be conjugated to B by a diagonal matrix whose diagonal entries are all ± 1 (i.e., by a *signing matrix*). We therefore adopt the following definition:

Definition 1.1. Given a graph G , we say that a graph H is an *inverse* of G if they possess adjacency matrices A_G and A_H such that A_H is signable to A_G^{-1} . We then say that G is *invertible*, and say that G is *simply invertible* if there exists a simple graph H which is an inverse of G . (In particular, we emphasize that a simple graph can be invertible but not simply invertible.)

Clearly this stronger condition defining invertibility implies the earlier reciprocal eigenvalue property, and it is thus easy to find non-invertible graphs – namely, any graph with an eigenvalue of 0, e.g., bipartite graphs on an odd number of vertices. In fact, this is a convenient place to note that for an invertible graph G with an inverse H , we must have $\det(A_G)^{-1} = \det(A_G^{-1}) = \det(A_H) \in \mathbb{Z}$, and so $\det(A_G) = \pm 1$ for any invertible graph. This forces G to admit a perfect matching (or “1-factor”), providing fairly compelling evidence that most graphs are not invertible. Following Godsil and the subsequent literature, we focus on graphs G which

¹“Graphs” in this article can include multiple edges between distinct vertices, but no loops. We will occasionally use the term multigraph when directly contrasting results to the corresponding properties for simple graphs.

are bipartite and have a *unique* perfect matching M . The first significant invertibility result ([4], Theorem 2.2) gives that a simple graph G (bipartite with a unique perfect matching M) is invertible if the graph G/M obtained by contracting each edge of M is bipartite. The aim of the current paper is to extend results of this form in a variety of different directions.

Summary of Results. Section 2 contains preliminaries on bipartite graphs with a unique perfect matching, focusing on inversion and extending previously well-known results for simple graphs to the context of multi-graphs. In particular, we give a purely graph-theoretic construction of the inverse (when it exists – see Theorem 2.5), which we dub the *parity closure* of the graph. We emphasize a graphical point of view (as opposed to a poset-theoretical or linear-algebraic one), enough so that it is frequently possible to bypass any matrix-inversion calculations and “eyeball” both the invertibility and inverse of a given graph. Further, we prove that the construction satisfies the desired properties of an inverse from the introduction (i.e., that $(G^{-1})^{-1} = G$ – see Theorem 2.9). In Section 3, we turn our attention to determining conditions for the inverse to exist. First, we extend a variety of known results on invertibility to the context of multigraphs, among them the result of Godsil mentioned above and a related result of [9] that a necessary condition for invertibility is the bipartiteness of a certain subgraph Γ of G/M . Continuing, we note that the main result of [9] gives much more, reducing the question of the invertibility of G to the invertibility of a collection of subgraphs (the “undirected intervals”) of G . Their culminating necessary and sufficient condition for invertibility admits some curiosities, however. If G is either:

- (a) A simply invertible undirected interval graph with bipartite Hasse diagram (Figure 1, left); or
- (b) A non-invertible interval graph with bipartite Hasse diagram all of whose proper sub-undirected intervals are invertible (Figure 1, right),

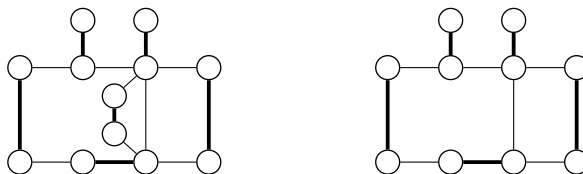


FIGURE 1.

then the principal result ([9], Theorem 2.6) returns a tautology – G is invertible if and only if G is invertible. The main result of Section 3 (Theorem 3.15) replaces undirected intervals with different key substructures which completely determine the invertibility of the graph, leading to a concise necessary and sufficient condition. In particular, Examples 3.18 and 3.19 determine the invertibility of the graphs in Figure 1 via a trivial calculation (especially in comparison to inverting and correctly signing a 12×12 or 10×10 matrix). As a more substantial application, we quickly recover the characterization of invertible unicyclic graphs found in [2]. We close the section focusing on the striking appearance of bipartiteness in the inversion results of both [4] and [9] and investigate the question of whether there exists an “optimal” subgraph of G/M in the sense that its bipartiteness is equivalent to the invertibility of G . We answer this in the negative but improve both previous results in the sense that we find a subgraph of G/M whose bipartiteness implies the invertibility of G , and a supergraph of Γ whose bipartiteness is implied by the invertibility of G (Theorems 3.24 and 3.27, respectively).

Finally, Section 4 addresses the question of how to construct invertible bipartite graphs with a unique perfect matching. If one views a graph as being constructed via a sequence of operations consisting of adding a new vertex and edges to that vertex, then it is natural to ask when such an operation preserves the invertibility of the graph. A complete answer to this question would provide a purely combinatorial description of the class of invertible graphs. Theorem 4.4 gives a necessary and sufficient condition for such an operation to preserve the invertibility of the graph, providing a rather large array of constructible classes of invertible graphs (see, e.g., Proposition 4.8.) As a demonstration of the utility, we return in Section 4.1 to the topic of unicyclic graphs, and describe explicit combinatorial constructions of invertible unicyclic graphs with prescribed size and cycle length.

2. PRELIMINARIES

As mentioned in the introduction, we restrict our attention to bipartite (multi-)graphs on $2n$ vertices with a unique perfect matching. We begin with a reduction process to simplify the discussion. First, any such graph can be visualized by arranging the edges of the perfect matching as vertical columns, with orientation chosen so that the top of each column is the same color (under some proper 2-coloring with colors, say, black and white). Next, uniformly orienting diagonal edges from black vertices to white vertices, we choose a topological sort of the columns so that the diagonal edges all have “positive slope,” as in the figure below. Finally, we construct the *digraph* $D = D_G$ associated to G by collapsing each vertical column to a single vertex. More precisely, D_G is the digraph whose vertices are the edges of the perfect matching with an edge from the i -th vertex to the j -th vertex of D_G if there is an edge from the bottom of the i -th column to the top of the j -th column in G . Figure 2 illustrates the construction of the associated digraph of a bipartite graph whose unique perfect matching is drawn in bold.

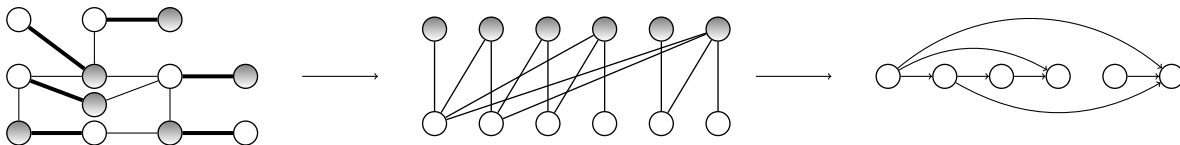


FIGURE 2. Construction of the associated digraph.

Note that the choice of topological sort will fix once and for all an ordering of the vertices of D , which we will consistently label by $\{1, 2, \dots, n\}$. If we now impose the labeling on G where the bottom row of vertices of G is $\{1, 2, \dots, n\}$ and the top row of vertices is $\{n + 1, \dots, 2n\}$, then the adjacency matrix $A = A_G$ of G has the simple block form

$$A = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix},$$

where B is the $n \times n$ matrix given by $B_{ii} = 1$ for all i , and for $i \neq j$, B_{ij} is the number of edges between columns i and j in G . The point of this construction is that the associated digraph D is a simpler object than G , yet contains all the information germane to its invertibility. Namely, since we have removed the matching edges when constructing D , its adjacency matrix is given by the upper-triangular matrix $B - I$. We have the following:

Theorem 2.1. *Given a bipartite multigraph G with unique perfect matching M , its adjacency matrix A is invertible with integral inverse matrix*

$$A^{-1} = \begin{bmatrix} 0 & (B^T)^{-1} \\ B^{-1} & 0 \end{bmatrix}.$$

Proof. The form of the inverse is readily verified by matrix multiplication. For the integrality condition, note that B is upper triangular with ones on the diagonal and so has determinant 1. By the inverse-adjugate formula, all the entries of B^{-1} are thus integers. \square

Recall from the introduction that by definition G is invertible if and only if A^{-1} is signable to the adjacency matrix of another graph, i.e., if there exists a (diagonal) signing matrix $S = (s_{ii})$, with $s_{ii} = \pm 1$ for all $1 \leq i \leq n$, such that $SA^{-1}S$ is an integral symmetric matrix with non-negative entries. Of course, since $SA^{-1}S$ is necessarily symmetric and integral, and $|(SA^{-1}S)_{ij}| = |(A^{-1})_{ij}|$, it suffices to check the existence of a signing matrix such that $SA^{-1}S = |A^{-1}|$, where $|A^{-1}|$ denotes the matrix obtained by taking absolute values of A^{-1} componentwise. Since we can conjugate block matrices by blocks, the matrix A^{-1} is signable if and only if the matrix B^{-1} is. If we abuse terminology slightly and say that D itself is *invertible* if B^{-1} is signable, we have now proved the following:

Theorem 2.2. *A bipartite graph G with unique perfect matching is invertible if and only if its associated digraph D is, i.e., if there exists a signing matrix S such that $SB^{-1}S = |B^{-1}|$.*

The problem of inverting G is thus reduced to the problem of signing B , and so we investigate the question of G 's invertibility through the lens of combinatorics on its associated digraph. As a first step in this direction, using the nilpotency of $B - I$, we can calculate the entries of B^{-1} via

$$B^{-1} = (I + (B - I))^{-1} = \sum_{m=0}^{\infty} (-1)^m (B - I)^m.$$

By standard results on adjacency matrices, $(B - I)_{i,j}^m$ counts the number of directed paths of length m between vertices i and j in D , and so the entries of B^{-1} are given by summing this quantity over all $m \geq 0$, each term weighted by ± 1 according to the parity of m :

$$(1) \quad B_{i,j}^{-1} = \#(\text{even-length paths from } i \text{ to } j \text{ in } D) - \#(\text{odd-length paths from } i \text{ to } j \text{ in } D).$$

Let $\mathcal{P}_{i,j} = \mathcal{P}_{i,j}(D)$ denote the set of all paths between vertices i and j in a digraph D , and $l(P)$ be the length of a path P . Equation (1) can be rewritten as

$$(2) \quad B_{i,j}^{-1} = \sum_{P \in \mathcal{P}_{i,j}(D)} (-1)^{l(P)}.$$

Remark 2.3. In the case that G is a *simple* graph, the above are special cases of poset-theoretical Möbius-inversion arguments. Namely, note that D can be thought of as defining a partial order on the set of vertices of G . Let P be this poset, and let ζ and μ be the Zeta and Möbius functions of this poset [1]. We have $B_{i,j} = \zeta(i, j)$ and $B_{i,j}^{-1} = \mu(i, j)$, and so inverting B amounts to being able to calculate $\mu(i, j)$ for each $i \leq j$ between 1 and n . Möbius inversion of ζ then gives the above formula.

Equation (2) hints to an explicit construction of a potential inverse. As a motivating example, consider the case that D is a directed tree, so that there is at most one path between any two vertices. In this case, $B_{i,j}^{-1} \in \{0, \pm 1\}$ for all i and j , with a non-zero value if and only if there is a directed path from i to j . Since any inverse to D should have exactly $|B_{i,j}^{-1}|$ edges from i to j , the upshot of this discussion is that the inverse should be a graph with an edge from i to j if and only if $B_{i,j} \neq 0$, i.e., if and only if there is a path from i to j in D . Such a graph is trivial to construct: In the figure below, a directed tree D is given with five (solid) edges, and its inverse is constructed by adding in the dashed edges.

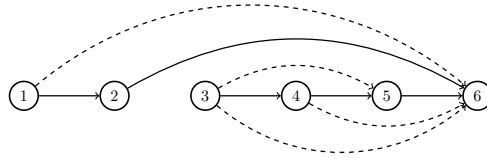


FIGURE 3. The inverse of a directed tree.

Note that this is the digraph corresponding to the transitive closure of the original digraph. Now if D admits (undirected) cycles, then Equation (3) is more complicated (e.g., two paths from i to j of opposite parity cancel each other out), but still describes a putative inverse via a “parity-corrected” transitive closure. We formalize this in a definition.

Definition 2.4. The *parity closure* of a digraph D is the directed graph D^+ on the vertices of D with exactly

$$\begin{aligned} |B_{i,j}^{-1}| &= |\#(\text{even-length paths from } i \text{ to } j \text{ in } D) - \#(\text{odd-length paths from } i \text{ to } j \text{ in } D)| \\ &= \left| \sum_{P \in \mathcal{P}_{i,j}(D)} (-1)^{l(P)} \right| \end{aligned}$$

edges from i to j for each $i < j$. If G is a bipartite graph with unique perfect matching and associated digraph D , we define G^+ to be the graph with adjacency matrix

$$A^+ = \begin{bmatrix} 0 & |(B^T)^{-1}| \\ |B^{-1}| & 0 \end{bmatrix}.$$

(Here again, $|B|$ denotes taking the componentwise absolute value of the matrix.)

We summarize the above discussion as the following theorem:

Theorem 2.5. *If D (resp. G) is invertible, then D^+ (resp. G^+) is its inverse.*

Remark 2.6. We remark that if one were to adopt the notation of G^{-1} for the inverse of G as in the introduction, the previous theorem could be re-phrased as the equality $G^+ = G^{-1}$ for invertible graphs G . In the sequel we will focus primarily on G^+ instead of G^{-1} as the former is defined for all graphs of interest.

Example 2.7. We complete in Figure 4 the process begun in Figure 2, constructing the parity closure of a bipartite graph G with a unique perfect matching. We form the associated digraph, take its parity closure (labels indicating multiple edges), and then return the graph to its original configuration. The dashed arrow on the left represents the composite process.

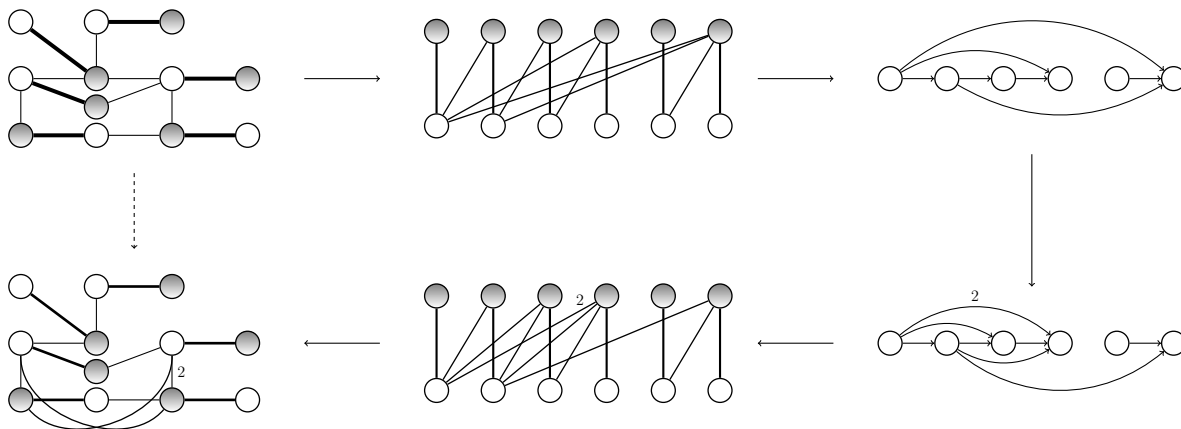


FIGURE 4. Constructing the parity closure of a bipartite graph with unique perfect matching

To emphasize, the constructed graph G^+ in the bottom-left is only the *potential* inverse of the original graph: There is no guarantee that the eigenvalues of G^+ are the reciprocals of those of G , but by Theorem 2.5, *if* the top-left graph is invertible, then this is indeed the case. Note then that the presence of the double edge in the parity closure immediately implies that the original graph is not simply invertible. Regardless, the key issue remaining is now to decide *a priori* the invertibility of a graph, a topic to which we devote the next section. In particular, we will see in Example 3.20 that the graph in Figure 4 is indeed invertible.

Before doing so, let us close the current section by remarking on the comment from the introduction that any reasonable notion of inversion should have the property that the double-inverse of a graph should be the original graph. We prove that this phenomenon does indeed occur with the parity closure.

Lemma 2.8. *If G is a bipartite graph with a unique perfect matching, then so is G^+ . In particular, G^{++} is defined.*

Proof. The block structure of A^+ provides the bipartition of G^+ and an easy induction argument proves that the unique perfect matching of G provides too the unique perfect matching of G^+ . \square

Theorem 2.9. *If G is an invertible bipartite graph with a unique perfect matching, then $G^{++} = G$.*

Proof. By Definition 2.4, the adjacency matrix of G^+ is $|A^{-1}|$. Since G is invertible, there exists a signing matrix S such that the adjacency matrix $|A^{-1}|$ of G^+ can be expressed $|A^{-1}| = SA^{-1}S$. By Lemma 2.8, G^{++} is defined, and we can consider its adjacency matrix $||A^{-1}|^{-1}| = |(SA^{-1}S)^{-1}| = |SAS|$. Since conjugation by S only changes the signs of the entries of A , $|SAS| = |A| = A$, and we have $G^{++} = G$. \square

If we dub graphs satisfying the condition $G^{++} = G$ as *reflexive*, it is natural to wonder about the converse to the theorem: Is every reflexive graph invertible? We conclude this section with a negative response to this question, via the reflexive non-invertible counter-example below. It would be interesting to characterize invertible graphs among reflexive graphs.

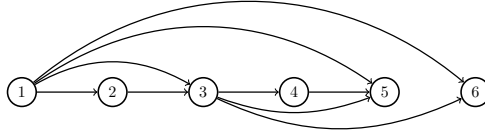


FIGURE 5. A non-invertible reflexive graph.

3. INVERTIBILITY

We maintain the notation from the previous section: D is a directed graph on $\{1, 2, \dots, n\}$ with adjacency matrix $B - I$. Our goal is to decide when D is invertible, i.e., when B^{-1} is signable to its absolute value $|B^{-1}|$, using the combinatorics of D . The following construction is of considerable interest.

Definition 3.1. Given a digraph D , let $\Gamma = \Gamma_D$ denote its *maximal-path subgraph*, the spanning subgraph of D which includes an edge e of D if and only if there exist vertices i and j of D such that e lies on a path from i to j whose length is maximal with respect to all such paths.

Remark 3.2. Roughly, Γ is the union, over all $i < j$, of all of the longest paths from i to j . It will be occasionally useful to adopt the equivalent but alternate point of view that Γ is constructed by deleting from D every edge e such that there exists a path in D of length greater than one connecting the endpoints of e . Thus we will often speak of edges of D “surviving to Γ ” if no such longer path exists.

The auxiliary graph Γ is used significantly in [9] (where it is named the Hasse Diagram of D , consistent with the poset-theoretic viewpoint therein) to prove the following necessary condition for invertibility. Our proof of the following result is essentially different only in notation and terminology from the original.

Theorem 3.3. *If B is signable, then Γ_D is bipartite.*

Proof. It is trivial to reduce to the case that Γ_D is connected, so we assume this is the case. Suppose there is a directed edge from i to j in Γ_D . By definition of Γ_D , this forces all directed paths from i to j in D to have length one, and thus by equation (1), $B_{i,j}^{-1} < 0$. If B^{-1} is signable, then considering the entry $(SB^{-1}S)_{i,j} = s_i B_{i,j}^{-1} s_j \geq 0$, we conclude that $s_i = -s_j$, i.e., entries corresponding to vertices connected by an edge of Γ_D must have opposite signs. By connectedness, arbitrarily setting $s_1 = +1$ (valid since S signs B^{-1} if and only if $-S$ does) now induces the sign of s_i for each vertex i . It is easy to see that grouping the vertices by this sign provides a bipartition of the vertices of Γ_D . \square

Definition 3.4. We introduce a pairing $\langle \cdot, \cdot \rangle : D \times D \rightarrow \{0, \pm 1\}$ on the vertices of D as follows: For $i, j \in D$, if P is a maximal-length path from i to j in D , let $l(P)$ denote its length, and set

$$\langle i, j \rangle = (-1)^{l(P)}.$$

If there are no paths from i to j in D , define $\langle i, j \rangle = 0$.

Lemma 3.5. *If Γ_D is bipartite and $i, j, k \in D$ are such that i is path-connected to j and j is path-connected to k , then*

$$\langle i, j \rangle \langle j, k \rangle = \langle i, k \rangle.$$

Proof. By bipartiteness, a longest path from i to j concatenated with a longest path from j to k must have the same parity as any (in particular, the longest) path from i to k . \square

We now have the following necessary and sufficient condition for invertibility.

Proposition 3.6. *If Γ_D is bipartite, then D is invertible if and only if for all $i, j \in D$ we have*

$$(3) \quad \langle i, j \rangle B_{i,j}^{-1} = \langle i, j \rangle \sum_{P \in \mathcal{P}_{i,j}(D)} (-1)^{l(P)} \geq 0.$$

Proof. The equality is the definition of $B_{i,j}^{-1}$, so the content of the proposition is the inequality. We assume without loss of generality that D is connected. For the first direction, assume $\langle i, j \rangle B_{i,j}^{-1} \geq 0$ for all i, j . Choose a coloring of Γ_D and let $s_i = +1$ if vertex i is colored black, and -1 otherwise. Now $s_i s_j$ is $+1$ if and only if i and j have the same color, which since Γ is bipartite and connected, occurs if and only if each (undirected) path from i to j has even length. Similarly, $s_i s_j = -1$ if each path, in particular any maximal-length path, has odd length. In other words, we have $s_i s_j = \langle i, j \rangle$. Now, letting S be the diagonal matrix whose diagonal entries are the s_i , we have

$$\langle i, j \rangle B_{i,j}^{-1} \geq 0 \implies s_i B_{i,j}^{-1} s_j \geq 0,$$

so D is invertible by Theorem 2.2. Conversely, assume that D is invertible. Then again by Theorem 2.2, there exists a signing matrix S such that $SB^{-1}S = |B^{-1}|$, i.e., integers $s_i = \pm 1$ such that $s_i B_{i,j}^{-1} s_j > 0$ for all i, j with $B_{i,j}^{-1} \neq 0$. If i and j are adjacent in Γ_D , then $\langle i, j \rangle = -1$, and $B_{i,j}^{-1} < 0$. Thus $s_i s_j = -1$, and we have $s_i s_j = \langle i, j \rangle$ for all pairs and (3) is satisfied. \square

Remark 3.7. Speaking loosely, the proposition tells us that a graph is invertible if and only if the *majority* of paths between any given pair of vertices have the same parity as the *longest* path between those two vertices. This is especially poignant, for example, when there are few paths between each pair of vertices (Corollary 3.16).

We note that the proposition is essentially equivalent to Corollary 5 in [2], which is proved using technical results from linear algebra. Our proof of this fact is self-contained and applies also to multigraphs. A motivating goal for the remainder of the section will be to improve this result by honing in on the crucial substructures which govern invertibility, in essence reducing the amount of calculation needed to determine the invertibility of the graph. Before doing so, let us extract from the proposition a few corollaries. The first of these is a generalization of Godsil's Theorem 1 ([4]) to multigraphs.

Corollary 3.8. *If D is bipartite, then D is invertible and D is a subgraph of D^+ .*

Proof. For arbitrary vertices i and j , the bipartiteness of D ensures that the lengths of all paths in $\mathcal{P}_{i,j}(D)$ have the same parity. Thus, every term in the sum $\sum_{P \in \mathcal{P}_{i,j}(D)} (-1)^{l(P)}$ has the same sign, and the same sign as $\langle i, j \rangle$. Therefore, by Theorem 3.6, D is invertible. Furthermore, $|B_{i,j}^{-1}|$ equals the number of paths between i and j , and thus $B_{i,j} \leq |B_{i,j}^{-1}|$, i.e., that D is a subgraph of D^+ . \square

Corollary 3.9. *If D is a simple, invertible graph and D^+ is bipartite, then D is simply invertible.*

Proof. Combining Theorem 2.9 and Corollary 3.8, D^+ is a subgraph of the simple graph $D^{++} = D$. \square

Lemma 3.10. *For any D , Γ_D is also a subgraph of D^+ (and hence of $D \cap D^+$).*

Proof. Suppose e is an edge from i to j in Γ_D . We prove that $B_{i,j}^{-1} \neq 0$, showing that there exists an edge from i to j in D^+ . Indeed, by definition of $B_{i,j}^{-1}$, the existence of an odd-length path from i to j in D (the path consisting of e alone) implies that if $B_{i,j}^{-1}$ were equal to zero, there would also be at least one even-length path from i to j in D . This contradicts that e lied on a maximal-length path in D . \square

Theorem 3.11. *For any D , the following are equivalent:*

- (i) D and D^+ are both bipartite.
- (ii) There is no path of length greater than one in D .
- (iii) $D = D^+$ and D is bipartite.

Proof. Clearly (i) follows directly from (iii). It remains to prove (i) \Rightarrow (ii) \Rightarrow (iii). First, (i) \Rightarrow (ii) : Suppose D and D^+ are bipartite and that there exists a path of length greater than one in D . Such a path ensures that there exist vertices i and j connected by an even length path in D . We conclude from this two consequences:

- The bipartiteness of D implies there is no odd path between i and j in D . Thus, by (3), $B_{i,j}^{-1} = \sum_{P \in \mathcal{P}_{i,j}(D)} (-1)^{l(P)} > 0$ and so vertices i and j are adjacent in D^+ .
- By definition of Γ_D and the bipartiteness of D , since there is an even length path between vertices i and j in D , then there is also an even length path between i and j in Γ_D . Since Γ_D is a subgraph of D^+ (Lemma 3.10), there is an even length path between adjacent vertices i and j in D^+ .

These two observations contradict that D^+ was assumed bipartite. Finally, we prove (ii) \Rightarrow (iii) : Suppose there does not exist a path of length greater than one in D . From the definition of parity closure, for any two vertices i and j , the number of edges from vertex i to vertex j in D^+ is

$$|\#(\text{even paths from } i \text{ to } j \text{ in } D) - \#(\text{odd paths from } i \text{ to } j \text{ in } D)|.$$

Since each such path is length 1, this simply returns the number of edges from i to j in D . Thus, $D = D^+$. Furthermore, the assumption that the length of all paths in D is less than or equal to 1 implies D is bipartite. \square

Our next corollary is the extension of the main theorem of Simion-Cao [8] to multigraphs. Here, we define a graph to be *self-dual* if $G = G^+$ and the *corona* of a graph H to be the graph obtained by adding to H a neighbor of degree 1 to each vertex.

Corollary 3.12. *A graph G is the corona of a bipartite multigraph H if and only if G is a self-dual bipartite multigraph with a unique perfect matching and bipartite D .*

Proof. Suppose G is the corona of a bipartite multigraph H . Clearly G inherits the bipartiteness of H and contains the unique perfect matching M consisting of the n pendant edges. Furthermore, since each edge of M contains a pendant vertex, each non-isolated vertex of D is either a source vertex or a sink vertex (i.e., can have vertices adjacent to it or is adjacent to other vertices, but not both). Thus D contains no paths of length greater than one. By Theorem 3.11, $D = D^+$ and D is bipartite.

The converse follows similarly: Suppose G is a bipartite multigraph with unique perfect matching M , D bipartite, and $G = G^+$. By Theorem 3.11, D does not contain a path of length greater than one. Thus each vertex of D is at most either a source or a sink (in particular, not both), and hence each edge in M contains a pendant vertex. Thus G is the corona of D . \square

3.1. Algorithm for Determining Invertibility. We begin with some combinatorial preliminaries on path-sets. For a graph D on vertices labelled $\{1, 2, \dots, n\}$ and a vertex $1 \leq k \leq n$, let $D - \{k\}$ be the subgraph of D resulting from the deletion of vertex k , retaining the original labels on all other vertices. Recall that for a digraph D , we denote by $B = B_D$ the upper uni-triangular matrix such that $B - I$ is the adjacency matrix of D . The following lemma relates the path-counting in D to that of $D - \{k\}$.

Lemma 3.13. *Suppose $i < k < j$ and let ${}_k B_{i,j}^{-1}$ denote the $(i, j)^{th}$ entry of $B_{D - \{k\}}^{-1}$. Then*

$$B_{i,j}^{-1} = B_{i,k}^{-1} B_{k,j}^{-1} + {}_k B_{i,j}^{-1}.$$

Proof. We abbreviate $\mathcal{P}_{i,j} = \mathcal{P}_{i,j}(D)$. If ${}_k \mathcal{P}_{i,j}$ denotes the set of paths from i to j *not* passing through k , then we have the decomposition $\mathcal{P}_{i,j} = (\mathcal{P}_{i,k} \times \mathcal{P}_{k,j}) \cup {}_k \mathcal{P}_{i,j}$, where we interpret an element of the product of the two path-sets as the concatenation of the two paths. Now by Equation (2), we have

$$\begin{aligned} B_{i,j}^{-1} &= \sum_{P \in \mathcal{P}_{i,j}} (-1)^{l(P)} = \sum_{P \in \mathcal{P}_{i,k}} \sum_{P' \in \mathcal{P}_{k,j}} (-1)^{l(P)+l(P')} + \sum_{P \in {}_k \mathcal{P}_{i,j}} (-1)^{l(P)} \\ &= \sum_{P \in \mathcal{P}_{i,k}} (-1)^{l(P)} \sum_{P' \in \mathcal{P}_{k,j}} (-1)^{l(P')} + \sum_{P \in {}_k \mathcal{P}_{i,j}(D - \{k\})} (-1)^{l(P)} \\ &= B_{i,k}^{-1} B_{k,j}^{-1} + {}_k B_{i,j}^{-1}. \end{aligned}$$

\square

We remark that the product structure induced from concatenation of paths is the key simplifying tool: a pair (i, j) has the property referenced at the start of the section – that there exists an intermediate vertex k such that every path from i to j passes through k – if and only if the set $\mathcal{P}_{i,j}$ can be written (“factors”) as the product of non-empty path-sets $\mathcal{P}_{i,k}$ and $\mathcal{P}_{k,j}$. This loose analogy between factoring integers and path-sets motivates the following terminology which will be of some use.

Definition 3.14. Given vertices i and j in D , we call the ordered pair (i, j) :

- a *zero pair* if there is no path in D from i to j ;
- a *unit pair* if all paths from i to j in D have length 1;
- a *composite pair* if there exists a vertex $k \in D$ with $i < k < j$ such that every path P from i to j in D passes through k ;
- a *prime pair* if it is neither a zero pair, a unit pair, nor a composite pair.

Finally, for graphs with Γ_D bipartite, we say the pair (i, j) is *signable* if $\langle i, j \rangle B_{i,j}^{-1} \geq 0$ and *simply signable* if $\langle i, j \rangle B_{i,j}^{-1} \in \{0, 1\}$. Note that under this definition of the signability of a pair, Proposition 3.6 says that a graph is invertible (resp. simply invertible) if and only if *all* pairs (i, j) are signable (resp. simply signable).

We turn to streamlining the results of Proposition 3.6. In particular, we look to significantly reduce the number of pairs (i, j) whose signability we need to evaluate in order to determine the invertibility of the graph. The rough strategy is to note that by Lemma 3.13, if all paths from i to j pass through an intermediate vertex k , then the signability of (i, j) is forced by the signability of the pairs (i, k) and (k, j) .

Theorem 3.15. *A digraph D is invertible (resp. simply invertible) if and only if Γ_D is bipartite and all prime pairs of D are signable. Similarly, a digraph D is simply invertible if and only if Γ_D is simple and bipartite and all prime pairs of D are simply signable.*

Proof. If D is invertible, then by Theorem 3.6 and Lemma 3.3, Γ_D is bipartite and

$$\langle i, j \rangle \sum_{P \in \mathcal{P}_{i,j}(D)} (-1)^{l(P)} = \langle i, j \rangle B_{i,j}^{-1} \geq 0$$

for all prime pairs (i, j) . For the converse, suppose that Γ_D is bipartite and that all prime pairs are signable, and let (i, j) be an arbitrary non-prime pair. If (i, j) is a zero pair, it is trivially signable, and if (i, j) is a unit pair, then $\langle i, j \rangle = -1$ and $B_{i,j}^{-1}$ is negative the number of edges from i to j , giving $\langle i, j \rangle B_{i,j}^{-1} > 0$. Finally, assume (i, j) is composite, so there exists a k with $i < k < j$ and $\mathcal{P}_{i,j} = \mathcal{P}_{i,k} \mathcal{P}_{k,j}$. Since no paths from i to j omit k , we have by Lemma 3.13 that $B_{i,j}^{-1} = B_{i,k}^{-1} B_{k,j}^{-1} + 0$. Recalling that prime pairs are signable, by induction we can assume that $\langle i, k \rangle B_{i,k}^{-1} \geq 0$ and $\langle k, j \rangle B_{k,j}^{-1} \geq 0$, and so

$$(4) \quad \langle i, j \rangle B_{i,j}^{-1} = \langle i, k \rangle B_{i,k}^{-1} \langle k, j \rangle B_{k,j}^{-1} \geq 0,$$

proving that in fact all pairs of D are signable. The claim for simple invertibility proceeds similarly: D is clearly simply invertible if and only if *all* pairs (i, j) are simply signable. It remains to show that it is sufficient to check the prime pairs. Since Γ_D is simple, all unit pairs are simply signable, and all zero pairs are trivially simply signable. If we assume all prime pairs are simply signable, then equation (4) shows that all composite pairs (and so all pairs) are simply signable, as desired. \square

This strengthening of Proposition 3.6 immediately decides the invertibility of some large classes of graphs.

Corollary 3.16. *If Γ_D is bipartite and if there are two or fewer paths between each prime pair (i, j) of D , then D is invertible.*

Proof. Note by definition of (i, j) being a prime pair, there cannot be zero or one paths from i to j . If there are two paths P and P' with, say, $l(P) \geq l(P')$, then

$$\langle i, j \rangle B_{i,j}^{-1} = (-1)^{l(P)} ((-1)^{l(P)} + (-1)^{l(P')}) = 1 + (-1)^{l(P)+l(P')} \geq 0.$$

Hence all prime pairs are signable. \square

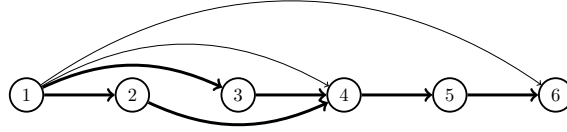
We include next a partial converse of Godsil’s Theorem:

Corollary 3.17. *A digraph D without prime pairs is invertible if and only if it is bipartite.*

Proof. By Theorem 3.15, D is invertible if and only if Γ_D is bipartite, but if D has no prime pairs, then $D = \Gamma_D$. \square

Before turning to some more involved examples, we observe that determining invertibility via even the reduced process of checking only prime pairs involves some redundant calculations. Specifically, since there can be substantial overlap in the computations needed for verifying the signability of a prime pair, we can avoid (or at least attempt to minimize) redundancy by attending first to prime pairs (i, j) with smaller values of $|j - i|$. Since we will wish to address the secondary question of when an invertible graph is additionally *simply* invertible, we note that in light of the second claim of Theorem 3.15 it is sufficient to check that $|B_{i,j}^{-1}| \leq 1$ for all prime pairs (i, j) . Recall that ${}_k B_{i,j}^{-1}$ denotes the $(i, j)^{th}$ entry of $B_{D-\{k\}}^{-1}$.

Example 3.18. This example determines the invertibility of the graph G in Figure 1 (left) from the introduction. Presented is the associated graph D , with its subgraph Γ_D consisting of the bold edges.



Since Γ_D contains no odd cycles, it is bipartite. The only prime pairs of D are $(1, 4)$ and $(1, 6)$. We have

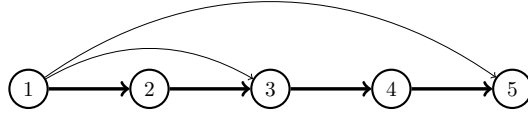
$$\langle 1, 4 \rangle B_{1,4}^{-1} = (-1)^2 (\#(\text{even paths from 1 to 4}) - \#(\text{odd paths from 1 to 4})) = 2 - 1 = 1 \geq 0,$$

so $(1, 4)$ is signable. By Lemma 3.13,

$$B_{1,6}^{-1} = B_{1,4}^{-1} B_{4,6}^{-1} + {}_4 B_{1,6}^{-1} = (1)(1) + (-1) = 0,$$

and so $(1, 6)$ is also signable. Further, since $|B_{i,j}^{-1}| \leq 1$ for both prime pairs, D (and hence G) is simply invertible.

Example 3.19. Similarly, below is the graph D for the graph G in Figure 1 (right) of the introduction. Again, the maximal-path subgraph Γ is drawn in bold.

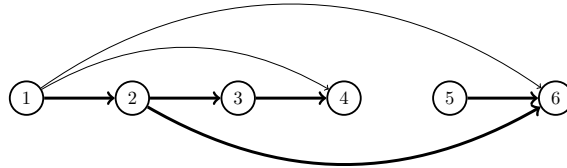


First we verify Γ_D is bipartite and note the only prime pairs are $(1, 3)$ and $(1, 5)$. We have $B_{1,3}^{-1} = 1 - 1 = 0$, but

$$\langle 1, 5 \rangle B_{1,5}^{-1} = (-1)^4 (B_{1,3}^{-1} B_{3,5}^{-1} + {}_3 B_{1,5}^{-1}) = (0)(1) + (-1) = -1,$$

so $(1, 5)$ is not signable, and G is not invertible.

Example 3.20. Finally, we reconsider the example of Figure 4, whose invertibility was left unanswered.



The only prime pairs are $(1, 4)$ and $(1, 6)$. By counting paths, we have

$$\langle 1, 6 \rangle B_{1,6}^{-1} = (-1)^2 (1 + (-1)) = 0$$

and

$$\langle 1, 4 \rangle B_{1,4}^{-1} = (-1)^3 (0 - 2) = 2 \geq 0,$$

so both prime pairs are signable. Hence G is invertible, but since $|B_{1,4}^{-1}| > 1$, it is not simply invertible.

3.2. Unicyclic graphs. Several authors have examined the invertibility of unicyclic bipartite graphs with a unique perfect matching. In [2], Akbari and Kirkland present necessary and sufficient criteria for the invertibility of such graphs. Below, we establish some preliminaries and derive their criteria from a prime pairs perspective. Briefly, the point is that a unicyclic graph can have at most one prime pair, so the methods from the last section are particularly apt. In Section 4.1, we present a new algorithm for constructing *all* invertible unicyclic bipartite graphs.

Let U be a unicyclic bipartite graph with unique perfect matching. The bipartiteness of U ensures that the cycle has even length, while the unique perfect matching forces the number of edges which are both in the perfect matching and incident to (and not in) the cycle to be even. Let $2m$ be the length of the cycle and $2k$ be the number of matched edges incident to the cycle. The topological sort of the vertices in Section 2 can be chosen to also consecutively order the matched edges in or incident to the cycle. The associated digraph D thus contains a single undirected cycle of length $m + k$, say on consecutive vertices $\{v + 1, \dots, v + (m + k)\}$, corresponding to the matched edges in or incident to the unicycle. Because a prime pair in any digraph produces an undirected cycle, the only possible prime pair in D is $(v + 1, v + m + k)$. Figure 6 shows a bipartite unicyclic graph with unique perfect matching and its associated digraph, with $m = 4$ and $k = 1$. Note that vertices $\{4, 5, 6, 7, 8\}$ form the undirected cycle of D .

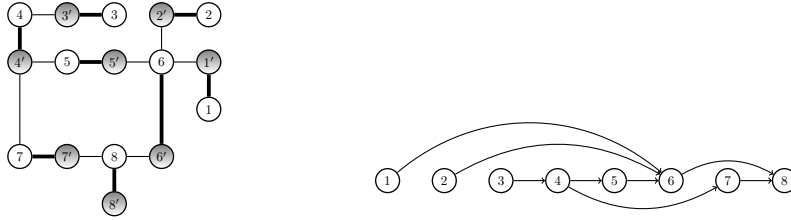


FIGURE 6. A bipartite unicyclic graph and its associated digraph.

In the following, we abuse terminology slightly and say that D is unicyclic if it is unicyclic as an undirected graph.

Lemma 3.21. *The pair $(v + 1, v + m + k)$ is prime if and only if $k = 1$.*

Proof. Let $i = v + 1$ and $j = v + m + k$. Consider the directed subgraph D' of D induced by the vertices $\{i, \dots, j\}$ corresponding to the matched edges in or incident to the unicycle in U . For all $w \in \{i, \dots, j\}$, w is a source or sink vertex in D' if and only if w corresponds to an incident matched edge. Thus, the number of source/sink vertices in D' is $2k$. The pair (i, j) forms a prime pair in D if and only if i is the only source and j is the only sink in D' , i.e., if and only if $k = 1$. \square

Theorem 3.22. *A unicyclic digraph D is invertible if and only if $m + k$ is even or $k = 1$ and the two matched edges incident to the unicycle are incident to adjacent vertices.*

Proof. Again let $i = v + 1$ and $j = v + m + k$, so that $\{i, \dots, j\}$ is the set of vertices forming an undirected cycle in D (listed in increasing order). Now $\Gamma_D = D$ unless (i, j) forms a prime pair and i is adjacent to j . Thus, by Lemma 3.21, if $k \neq 1$ or i is not adjacent to j , and $m + k$ is odd, then $\Gamma_D = D$ and contains an odd cycle of length $m + k$. By Theorem 3.3, D is not invertible.

If $m + k$ is even, or $k = 1$ and vertices i and j are adjacent, then Γ_D either contains only an even cycle or Γ_D is the acyclic graph formed by deleting the edge between i and j in D . In either case, Γ_D is bipartite. The unicyclicity of D ensures there are two or fewer paths between the only possible prime pair (i, j) . Thus, D is invertible by Corollary 3.16. \square

Corollary 3.23. *An invertible unicyclic graph D is simply invertible if and only if $k > 1$ or $m + k$ is odd.*

Proof. If $k = 1$ then there are exactly two paths between the only prime pair vertices i and j . If those paths are of the same parity (i.e., if $m + k$ is even) then $|B_{i,j}^{-1}| = 2$ and D is not simply invertible. If those paths are of opposite parity (i.e., $m + k$ is odd) then $|B_{i,j}^{-1}| = 0$ and D is simply invertible. If $k > 1$ then D contains no prime pairs and $|B_{x,y}^{-1}| \leq 1$ for all vertices x, y in D . \square

3.3. Optimal Bipartite Subgraph. We finish this section with an attempt to unite the two striking links between invertibility and bipartiteness found in [4] and [9], and their generalization to multigraphs (Corollary 3.8 and Theorem 3.3). Namely, we have that for a directed graph D :

- If D is bipartite, D is invertible.
- If D is invertible, Γ_D is bipartite.

One is led to wonder the extent to which these two results are optimal, i.e., ask:

- Are there proper subgraphs of D whose bipartiteness implies the invertibility of D ?
- Are there proper supergraphs of Γ_D whose bipartiteness is implied by the invertibility of D ?

The answers to these can be trivially negative for a *given* graph (e.g., take any invertible graph such that $D = \Gamma_D$), so we mean to ask these in the broader context of canonical constructions that have the potential of being proper subgraphs and supergraphs, respectively. In particular, it is natural to ask if there is a canonically-defined subgraph H_D of D satisfying $\Gamma_D \leq H_D \leq D$ whose bipartiteness is equivalent to the invertibility of D . In this context, we answer both of the bulleted question in the affirmative, but conclude that such a “bipartite litmus test” does not exist. Let us first improve the “upper bound” $H_D \leq D$.

Theorem 3.24. *Suppose $(i_1, j_1), (i_2, j_2), \dots, (i_n, j_n)$ are prime pairs of D such that for all k :*

- $j_k \leq i_{k+1}$ for $1 \leq k \leq n-1$.
- There is an edge e_k from i_k to j_k in D .

Let D' be the graph obtained from D by deleting e_k , for $1 \leq k \leq n$. Then if D' is bipartite, D is invertible.

Proof. By assumption, the removed edges e_k did not survive to Γ_D , so Γ_D is a subset of D' . In particular, since D' is assumed bipartite, Γ_D is as well, and so we need only to check that each prime pair (a, b) of D is signable. We partition the set $\mathcal{P} = \mathcal{P}_{a,b}(D)$ of paths from a to b in D according to which of the pairs (i_k, j_k) a path goes through, i.e., writing

$$\mathcal{P} = \bigcup_{S \subset \{1, 2, \dots, n\}} \mathcal{P}_S,$$

where \mathcal{P}_S is the subset of \mathcal{P} consisting of paths that pass through both i_k and j_k for exactly those $k \in S$ (of course, S can be empty). This induces an analogous decomposition of $B_{a,b}^{-1}$:

$$\langle a, b \rangle B_{a,b}^{-1} = \langle a, b \rangle \sum_{P \in \mathcal{P}} (-1)^{l(P)} = \sum_{S \subset \{1, 2, \dots, n\}} \langle a, b \rangle \sum_{P \in \mathcal{P}_S} (-1)^{l(P)}.$$

It suffices to show that each of these summands is non-negative. Write $S = \{m_1, \dots, m_k\}$, so that

$$\mathcal{P}_S = \mathcal{P}_{a, i_{m_1}} \times \mathcal{P}_{i_{m_1}, j_{m_1}} \times \mathcal{P}_{j_{m_1}, i_{m_2}} \times \mathcal{P}_{i_{m_2}, j_{m_2}} \times \dots \times \mathcal{P}_{j_{m_{k-1}}, i_{m_k}} \times \mathcal{P}_{i_{m_k}, j_{m_k}} \times \mathcal{P}_{j_{m_k}, b}.$$

Setting $j_{m_0} = a$ and $i_{m_{k+1}} = b$ for notational convenience (if not aesthetics), we find

$$\langle a, b \rangle \sum_{P \in \mathcal{P}_S} (-1)^{l(P)} = \prod_{\alpha=0}^k \langle j_{m_\alpha}, i_{m_{\alpha+1}} \rangle B_{j_{m_\alpha}, i_{\alpha+1}}^{-1} \prod_{\alpha=1}^k \langle i_{m_\alpha}, j_{m_\alpha} \rangle B_{i_{m_\alpha}, j_{m_\alpha}}^{-1}.$$

Here we have used Lemma 3.5. Finally, we check that each of the factors above is positive:

- (1) Since the path-sets $\mathcal{P}_{j_{m_\alpha}, i_{m_{\alpha+1}}}$ remain unchanged by the deletion of the e_k 's, the corresponding factors can be written as follows:

$$\langle j_{m_\alpha}, i_{m_{\alpha+1}} \rangle B_{j_{m_\alpha}, i_{\alpha+1}}^{-1}(D) = \langle j_{m_\alpha}, i_{m_{\alpha+1}} \rangle B_{j_{m_\alpha}, i_{\alpha+1}}^{-1}(D').$$

Now each of these are positive since D' is bipartite, making every pair $(j_{m_\alpha}, i_{m_{\alpha+1}})$ signable.

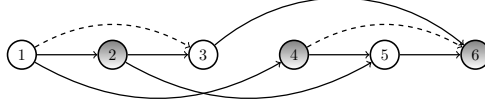
- (2) Since the path sets $\mathcal{P}_{i_{m_\alpha}, j_{m_\alpha}}(D)$ and $\mathcal{P}_{i_{m_\alpha}, j_{m_\alpha}}(D')$ differ by the single edge e_{m_α} , the remaining factors satisfy

$$\langle i_{m_\alpha}, j_{m_\alpha} \rangle B_{i_{m_\alpha}, j_{m_\alpha}}^{-1} = \langle i_{m_\alpha}, j_{m_\alpha} \rangle B_{i_{m_\alpha}, j_{m_\alpha}}^{-1}(D') \pm 1 \geq 0,$$

where we have used that by virtue of signability and having at least one other path between them, $\langle i_{m_\alpha}, j_{m_\alpha} \rangle B_{i_{m_\alpha}, j_{m_\alpha}}^{-1}(D')$ is positive and at least one. □

Remark 3.25. We note that if $D \neq \Gamma_D$, then one can find prime pairs as in the theorem, thereby constructing a *proper* subgraph D' of D whose bipartiteness implies the invertibility of D .

Example 3.26. The figure below gives a (non-bipartite) digraph the demonstration of whose invertibility requires a moderate calculation using the techniques of Section 3.1, but which is trivial in light of the previous theorem. Namely, applying the theorem to the prime pairs $(1, 3)$ and $(4, 6)$, we see that the deletion of the dashed edges leaves a bipartite graph (with bipartition given by the shading). Theorem 3.24 now allows us to conclude the original graph is invertible.



In the other direction, we wish to improve the “lower bound” $\Gamma_D \leq H_D$, i.e., to find a supergraph of Γ_D whose bipartiteness is forced by the invertibility of D .

Theorem 3.27. *Let Δ_D be the subgraph of D obtained by removing every edge e_{ij} connecting vertices i and j with $\langle i, j \rangle = 1$. Then Δ_D is bipartite if D is invertible.*

Proof. If D is invertible, then Γ_D is bipartite. Let $l(i, j)$ denote the length of the maximal path from i to j in D (or Γ_D), and note that Γ_D is formed from D by removing any edge e_{ij} not on a maximal-length path from i to j , i.e., removing e_{ij} if $l(i, j) > 1$. Since Δ_D is formed from D by removing edges e_{ij} with $l(i, j)$ even, one can alternatively view Δ_D as being constructed as the supergraph of Γ_D where one adds back in an edge e_{ij} from D if and only if $l(i, j)$ is odd and greater than 1. But adding an edge between vertices with $\langle i, j \rangle = -1$ can never construct an odd cycle, so the bipartiteness of Γ_D forces the bipartiteness of Δ_D as well. \square

Remark 3.28. Analogously to Remark 3.25, we note that if D is invertible and not itself bipartite, then Δ_D is a *proper* bipartite supergraph of Γ_D .

As above, it is of clear interest to ask if these bounds can be tightened so as to uniquely identify a canonical subgraph of a general D whose bipartiteness is equivalent to the invertibility of D . Without attempting to make this question particularly precise, we note that the proof of the previous theorem convincingly prohibits such a subgraph from existing. Namely, Δ_D is quite clearly maximal with respect to the property given in the theorem – any supergraph of Δ_D in D contains an edge e_{ij} between a pair of vertices with $\langle i, j \rangle = 1$ and hence is not bipartite. Thus the only candidates for an “optimal bipartite subgraph” are subgraphs of Δ_D , so a single example of a non-invertible graph with bipartite Δ_D proves the impossibility of a subgraph whose bipartiteness is equivalent to the invertibility of D . We furnish such an example below:

Example 3.29. Let D be the graph in Figure 7. Then D is non-invertible, since the prime pair $(1, 4)$ is not signable (we have $\langle 1, 4 \rangle B_{1,4}^{-1} = (-1)(2 - 1) = -1$), but Δ_D , obtained by removing the dashed edges, is clearly bipartite. We also note that Δ_D is a proper supergraph of Γ_D in this example, since the edge $e_{2,5} \in \Delta_D - \Gamma_D$.

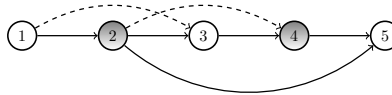


FIGURE 7. A non-invertible graph with bipartite Δ_D

4. CONSTRUCTING INVERTIBLE BIPARTITE GRAPHS WITH UNIQUE PERFECT MATCHING

We begin by introducing some notation. For vertices $d, d' \in D$, write $d \rightarrow d'$ if there is a directed edge from d to d' , and $d \rightsquigarrow d'$ if there is a directed path from d to d' . Recall that by our conventions on labeling, our directed graphs have the property that if $d \rightarrow d'$, then $d < d'$. In this section we present an algorithm for constructing all invertible digraphs, and hence all invertible bipartite graphs with unique perfect matching. We begin with the following straight-forward proposition:

Proposition 4.1. *All digraphs having the property that $d < d'$ whenever $d \rightarrow d'$ can be constructed from the graph on a single vertex (labelled 1), via a sequence of operations of the form:*

If D has vertices $\{1, 2, \dots, n-1\}$, choose a subset $S_n \subseteq \{1, 2, \dots, n-1\}$ and add a vertex labelled n and (possibly multiple) adjacencies $s \rightarrow n$ for all $s \in S_n$.

To construct all *invertible* digraphs, we find necessary and sufficient conditions on the set S in the proposition to ensure invertibility at each stage of the construction process. This is clearly a requirement for the invertibility of the resulting graph. If any intermediate graph D of the construction process is non-invertible then either the associated graph Γ_D is not bipartite or D contains an unsignable prime pair. Since neither of these deficiencies can be rectified by the above process of adding further vertices and/or edges, if at any stage of the construction process the resulting graph is non-invertible, the final resulting graph will be non-invertible.

Definition 4.2. Given a subset S of (the vertices of) an invertible directed graph D (on vertex set $\{1, 2, \dots, n-1\}$), let D_S denote the graph obtained by adjoining a new vertex labeled n to D and adding edges $s \rightarrow n$ for each $s \in S$. Call $t \in S$ *terminal* if $t \not\rightarrow s$ for all $s > t$ in S . Call S *valid* if the maximal-path subgraph Γ_{D_S} is bipartite.

Lemma 4.3. *A subset S of an invertible digraph D is valid if and only if $\langle t, n \rangle = -1$ in D_S for all terminal $t \in S$.*

Proof. Since D is invertible, Γ_D is bipartite. If t is terminal, then there exists a unique path from t to n in D_S , namely the length-one path $t \rightarrow n$. Since this path necessarily survives to the maximal-path subgraph, we must have $\langle t, n \rangle = -1$. On the other hand, if s is non-terminal, then the edge $s \rightarrow n$ is not an edge of the maximal-path subgraph, and thus has no bearing on the bipartiteness of Γ_{D_S} . \square

Theorem 4.4. *Let S be a valid subset of an invertible graph D . For a vertex $d \in D$, define $S_d = \{s \in S \mid d \rightsquigarrow s\}$, and partition S_d into two sets S_d^+ and S_d^- according to whether $\langle s, n \rangle = \pm 1$. Then D_S is invertible iff for all $d \in D$ with $|S_d| \geq 2$, we have*

$$(5) \quad \sum_{s \in S_d^-} |B_{d,s}^{-1}| \geq \sum_{s \in S_d^+} |B_{d,s}^{-1}|.$$

Proof. Since D is invertible, all prime pairs not including n are already signable, so by Theorem 3.15, it suffices to check the prime pairs involving n , namely those prime pairs (d, n) with $|S_d| \geq 2$. Write $S_d = \{s_1, \dots, s_k\}$. Repeatedly using the fact that s_{j-1} is terminal in $D - \{s_j, s_{j+1}, \dots, s_k\}$, we have

$$\begin{aligned} B_{d,n}^{-1} &= B_{d,s_k}^{-1} B_{s_k,n}^{-1} + s_k B_{d,n}^{-1} \\ &= -B_{d,s_k}^{-1} + s_k B_{d,s_{k-1}}^{-1} \cdot s_k B_{s_{k-1},n}^{-1} + s_k B_{d,n}^{-1} \\ &= \vdots \\ &= -B_{d,s_k}^{-1} - B_{d,s_{k-1}}^{-1} - \dots - B_{d,s_1}^{-1} \\ &= -\sum_{j=1}^k B_{d,s_j}^{-1}. \end{aligned}$$

Now use $\langle d, n \rangle B_{d,n}^{-1} = \langle d, s_j \rangle \langle s_j, n \rangle B_{d,s_j}^{-1} = \langle s_j, n \rangle |B_{d,s_j}^{-1}|$ by signability of (d, s_j) to get

$$\langle d, n \rangle B_{d,n}^{-1} = -\langle d, n \rangle \sum_{s \in S_d} B_{d,s}^{-1} = -\sum_{s \in S_d} \langle d, s \rangle \langle s, n \rangle B_{d,s}^{-1} = -\sum_{s \in S_d} \langle s, n \rangle |B_{d,s}^{-1}| = \sum_{s \in S_d^-} |B_{d,s}^{-1}| - \sum_{s \in S_d^+} |B_{d,s}^{-1}|,$$

whose positivity is the statement of the theorem. \square

Corollary 4.5. *Let D and S be as in the theorem. If D can be colored so that S is monochromatic, then D_S is invertible.*

Proof. We have $\langle s, n \rangle = -1$ for all $s \in S$, so S_d^+ is empty and the inequality (5) is trivially satisfied. \square

As a corollary, we can immediately recover again the result of Godsil:

Corollary 4.6. *If D is bipartite, it is invertible.*

Proof. If D is bipartite, it can be constructed by a sequence of iterations of the construction given above, adding a new right-most vertex and connecting to a subset S of the vertices, all of the same color. \square

Corollary 4.7. *Let D and S be as in the theorem. If $|S| = 1$, then D_S is invertible.*

Proof. Since $|S| = 1$, there are no $d \in D$ with $|S_d| \geq 2$, so the condition is vacuously satisfied. \square

Non-monochromatic sets S do not appear to admit particularly simple conditions for guaranteeing the invertibility of D_S . The next proposition deals with the case $|S| = 2$.

Proposition 4.8. *Let $S = \{s, s'\}$ be a valid subset of an invertible graph D . Then D_S is invertible unless (and only unless) $\langle s, s' \rangle = -1$, $s \rightsquigarrow s'$, and there exists $d \in D$ path-connected to both s and s' such that*

$$|B_{d,s'}^{-1}| < |B_{d,s}^{-1}|.$$

In particular, if $s = 1$, then D_S is invertible.

Proof. First, if $\langle s, s' \rangle = 1$, then D_S is invertible by Corollary 4.5. We thus assume that $\langle s, s' \rangle = -1$. Further, we may assume that $s \rightsquigarrow s'$, since otherwise the subset $\{s, s', n\} \subset \Gamma_{D_S}$ could not be 2-colored, contradicting our assumption that S was valid. Since D is invertible, it suffices to check the new prime pairs created upon addition of n , which are exactly the prime pairs (d, n) for d such that $d \rightsquigarrow s$. For such d , we have $S_d = \{s, s'\}$, independently of d . Since $\langle s, n \rangle = 1$, and $\langle s', n \rangle = -1$, Theorem 4.4 gives that D_S is invertible if and only if $|B_{d,s'}^{-1}| \geq |B_{d,s}^{-1}|$ for each such d . \square

Corollary 4.9. *Let $S = \{s, s'\}$ be a valid subset of an invertible graph D . Then there exists a positive integer k such that if k edges are added to D connecting s to s' , then D_S is invertible.*

Proof. From the proposition, D_S is invertible if for all d path-connected to both s and s' , we have $|B_{d,s'}^{-1}| \geq |B_{d,s}^{-1}|$. Writing $B_{d,s'}^{-1} = B_{d,s}^{-1}B_{s,s'}^{-1} + {}_sB_{d,s'}^{-1}$ and canceling a $B_{d,s}^{-1}$ from both sides (if $B_{d,s}^{-1} = 0$, the inequality is trivially satisfied), we arrive at the invertibility condition

$$\left| \frac{{}_sB_{d,s'}^{-1}}{B_{d,s}^{-1}} + B_{s,s'}^{-1} \right| \geq 1.$$

Since $B_{s,s'}^{-1}$ is independent of d , one can ensure that this inequality is satisfied for all such d by choosing, for example,

$$B_{s,s'}^{-1} \geq 1 + \max_{d: B_{d,s}^{-1} \neq 0} \left| \frac{{}_sB_{d,s'}^{-1}}{B_{d,s}^{-1}} \right|.$$

\square

4.1. Application: Constructing invertible unicyclic graphs. As an extended example of the iterative construction process, we turn our attention to directed graphs D which are associated to bipartite unicyclic graphs with a unique perfect matching (and in particular, invertible such digraphs). As in the previous section, we begin with a single vertex D_1 and iteratively adjoin edges to new vertices. More precisely, we proceed inductively for $i \geq 2$, letting D_i be the graph obtained by adding a new vertex i to D_{i-1} , and edges $s \rightarrow i$ for all s in some *adjacency set* $S_i \subseteq [1, i-1]$. Given adjacency sets S_1, \dots, S_n , we will often denote simply by D rather than D_n the end result of iteratively adjoining each S_i .

We break the construction of all unicyclic graphs into two steps: first the construction of the cycle, and then the rest of the graph. The idea in both steps is to precisely describe the combinatorial restrictions on the number of edges added at each stage of the iteration (i.e., on $|S_i|$) forced by unicyclicity. To this end, we introduce the following terminology:

Definition 4.10. A *Motzkin partition* of a positive integer N is a partition $P = \{p_1, \dots, p_N\}$ of N into exactly N parts such that $0 \leq p_i \leq 2$ for all i , and $\sum_{k=1}^i p_k < i$ for all $i < N$. Note that the partial sum condition forces $p_1 = 0$ and $p_N = 2$.

Remark 4.11. We so-name these partitions due to their connection to the well-known Motzkin numbers (e.g., [6], sequence A001006). The authors wish to thank David Speyer [7] for pointing out this link to us. We note that a previous combinatorial interpretation of Motzkin numbers in terms of unicyclic graphs does not seem to exist in the literature (see, e.g., [3]).

Continuing our slight abuse of terminology from Section 3.2, we say that a digraph D is the cycle graph (resp. unicyclic or acyclic) if it is the cycle graph (resp. unicyclic or acyclic) as an undirected graph. We begin by describing the possible iterative constructions of the cycle graph on N vertices. To avoid conflicting with future notation, we use C_i instead of S_i to describe the adjacency sets for the cycle.

Proposition 4.12. *Let P be a Motzkin partition of N . Then there exist adjacency sets $C_i \subseteq [1, i - 1]$ for $2 \leq i \leq N$, such that $|C_i| = p_i$ and such that the digraph D resulting from iteratively adjoining these adjacency sets is the cycle graph on N vertices.*

Proof. We will construct sets C_i for $2 \leq i \leq n$ such that $|C_i| = p_i$ and such that the resulting graph D is two-regular and connected. From this it easily follows that, as an undirected graph, D is the cycle on $\sum p_i = N$ vertices. As always, let D_1 denote the single-vertex graph. We proceed inductively, for $i \geq 2$ choosing $C_i \subset [1, i - 1]$ of size p_i and letting D_i be obtained from D_{i-1} by adding vertex i and edges $c \rightarrow i$ for each $c \in C_i$. Note that to prove D is two-regular and connected it is necessary and sufficient to prove that we can choose our adjacency sets such that D_i is acyclic for all $i < N$, and has maximum vertex degree at most 2 for all i . These properties are clearly satisfied by D_1 . Now the induction: Suppose that D_i ($1 \leq i \leq N - 2$) is acyclic with maximum vertex degree at most 2. We show that we can choose C_{i+1} so that $|C_{i+1}| = p_{i+1}$ and D_{i+1} again is acyclic with maximum vertex degree at most 2. If $p_{i+1} = 0$, this is trivial. If $p_{i+1} = 1$, we simply need to prove the existence of a vertex of degree at most 1 in D_i : If such a vertex did not exist, we would have $\sum_{k=1}^i p_k = i$, contradicting the partial sum condition of Motzkin partitions. Similarly, if $p_{i+1} = 2$ and there are not two unconnected vertices of degree at most one, then D_i is the path graph on i vertices and we have $\sum_{k=1}^i p_k = i - 1$. But now $\sum_{k=1}^{i+1} p_k = i - 1 + 2 = i + 1$, again violating the partial sum condition. Thus for all $i < N$ we can select the desired adjacency sets C_i . \square

Next we show how to iteratively construct all graphs with a prescribed number of vertices M and a unique cycle on a prescribed set of N vertices. From this it is easy to see that we can so construct all unicyclic graphs (Remark 4.15). Recall that by choosing a different topological sort if necessary, we can assume that the cycle occurs on consecutive vertices, say on vertices $\{v + 1, \dots, v + N\}$. The apparent combinatorial complexity of the following proposition is a result of having to choose adjacency sets S_i so that they include the sets C_i as above (thus constructing a cycle of the desired length), while ensuring that a second cycle is never created.

Proposition 4.13. *Let M and N be positive integers with $M > N$, and let v be an integer between 1 and $M - N$. Let $P = \{p_{v+1}, \dots, p_{v+N}\}$ be a Motzkin partition of N and $T = \{t_1, \dots, t_M\}$ be a partition of M into M parts such that*

- $t_i \geq p_i$ for all $v + 1 \leq i \leq v + N$;
- $\sum_{k=1}^i t_k \leq i$ for all i ;
- $\sum_{k=1}^i t_k < i$ for all $1 \leq i < v + N$.

Then there exist adjacency sets $S_i \subset [1, i - 1]$ of size t_i , for $1 < i \leq M$, such that the digraph D resulting from the iterative construction process has M vertices, M edges, and a single undirected cycle of length N on vertices $v + 1$ through $v + N$.

Proof. For the proof of this proposition, we consider a slight alteration to the construction process. Instead of adjoining a new vertex i at the i -th step, we begin with the completely disconnected graph on M vertices and, for $1 < i \leq M$, consider adding the directed edges $s \rightarrow i$ for all s in the adjacency set S_i . Define the partition $Q = \{q_1, \dots, q_M\}$ of $M - N$ into M parts by

$$q_i = \begin{cases} t_i - p_i & \text{for } v + 1 \leq i \leq v + N \\ t_i & \text{else} \end{cases}.$$

By Proposition 4.12, for $v + 1 < i \leq v + N$ there exist adjacency sets C_i such that $|C_i| = p_i$ and the graph resulting from adding the edges $c \rightarrow i$ for all c in C_i and all $v + 1 < i \leq v + N$ is the cycle graph on vertices

$\{v + 1, \dots, v + N\}$. We will prove the existence of sets S_i ($1 < i \leq M$), by showing the existence of sets R_i with $|R_i| = q_i$, and setting $S_i = R_i \cup C_i$ (here $C_i = \emptyset$ for all $i \notin [v + 2, v + N]$). Create the graph on M vertices consisting of a single cycle on vertices $\{v + 1, \dots, v + N\}$ by adding the directed edges $c \rightarrow i$ prescribed by the adjacency sets C_i for $v + 1 < i \leq v + N$. Call this graph H_1 . For $1 < i \leq M$, let H_i denote the graph obtained from H_{i-1} by adding edges $s \rightarrow i$ for all $s \in R_i$. Assuming the graph H_{i-1} is unicyclic, it remains to show that in the i -th step we can select the q_i vertices of R_i such that the resulting graph is unicyclic., i.e., that the part of the graph to the left of i has at least q_i connected components. For ease of notation, we split into several cases.

Case I ($1 < i \leq v$): Let h_i be the number of connected components of $H_{i-1} \cap [1, i - 1]$. Since there are no cycles in $H_{i-1} \cap [1, i - 1]$, we have $h_i = i - 1 - \sum_{k=1}^{i-1} q_k$. The condition that there are sufficiently many connected components in constructing H_i is simply $q_i \leq h_i$, i.e., that $\sum_{k=1}^i q_k \leq i - 1 < i$, but this is true by assumption (noting $q_k = t_k$ for $k < v$).

Case II ($v + 1 \leq i \leq v + N$): Since any additional edge between two vertices of the cycle would force a second cycle, for vertices in the range $[v + 1, v + N]$, it suffices to show that for each such i , the number of connected components in $H_{i-1} \cap [1, v + N]$, given by $h_i = v + 1 - \sum_{k=1}^{i-1} q_k$, is at least $q_i + 1$ (the cycle accounts for the extra connected component). Again, this is equivalent to the condition that $\sum_{k=1}^i q_k \leq v$, which follows from

$$\sum_{k=1}^i q_k \leq \sum_{k=1}^{v+N} q_k = \sum_{k=1}^{v+N} t_k - N \leq v + N - N.$$

Case III ($v + N + 1 \leq i \leq M$): For $i > v + N$, the number of connected components in $H_{i-1} \cap [1, i - 1]$ is calculated by considering the v initial vertices, the cycle, and the $i - (v + N) - 1$ vertices between $v + N$ and i (i.e. the number of vertices between the cycle and i). Each of the $\sum_{k=1}^{i-1} q_k$ added edges joins two of these components. Thus the number of connected components in $H_{i-1} \cap [1, i - 1]$ is

$$h_i = v + 1 + i - (v + N) - 1 - \sum_{k=1}^{i-1} q_k = i - N - \sum_{k=1}^{i-1} q_k,$$

and the unicyclicity condition is just $q_i \leq i - N - \sum_{k=1}^{i-1} q_k$. Equivalently, we need $\sum_{k=1}^i q_k \leq i - N$, which follows from

$$\sum_{k=1}^i q_k = \sum_{k=1}^i t_k - N \leq i - N.$$

□

We illustrate this construction process with the following example.

Example 4.14. Let $M = 8$ and $N = 5$ and $v = 2$. The following partitions meet the requirements of Proposition 4.12 and 4.13:

$$T = \{0, 1, 0, 0, 2, 2, 2, 1\} \quad P = \{0, 0, 2, 1, 2\}.$$

To begin, we construct the cycle on vertices $\{3, 4, 5, 6, 7\}$. By the requirement that $|C_i| = p_i$, the fact that $p_3 = p_4 = 0$ forces the adjacency sets C_3 and C_4 to be empty. The only possible choices for C_5 is then $\{3, 4\}$. There are two valid options for the set C_6 , namely $\{3\}$ or $\{4\}$. C_7 is determined by our choice for C_6 , with $C_7 = \{4, 6\}$ if $C_6 = \{3\}$ and $C_7 = \{3, 6\}$ otherwise. Thus, there are two possibilities for the intermediate graph H_1 consisting of just the cycle, as shown in Figure 4.14.

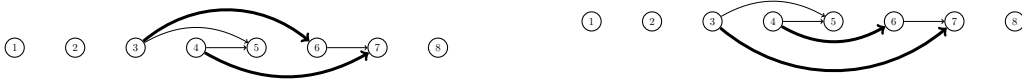


FIGURE 8. Two possible intermediate digraphs H_1 resulting from the iterative construction process on partition $P = \{0, 0, 2, 1, 2\}$, with $M = 8$ and $v = 2$.

Since $|S_i| = t_i$, S_3 , and S_4 are the empty set. The only possible non-empty adjacency set for S_2 is $\{1\}$. For $3 \leq i \leq 7$, $C_i \subseteq S_i$. By our definitions of P and T , $|S_5| = |C_5|$, $|S_7| = |C_7|$, and $|S_6| = |C_6| + 1$. Thus, sets S_5 and S_6 are completely determined by H_1 , while S_6 contains the subset C_6 and one additional vertex chosen from $\{1, 2\}$. The final adjacency set S_8 can equal any single vertex in the set $\{1, 2, \dots, 7\}$. Figure 9 shows the two possible resulting digraphs if we set $S_6 = C_6 \cup \{2\}$ and $S_8 = \{7\}$.

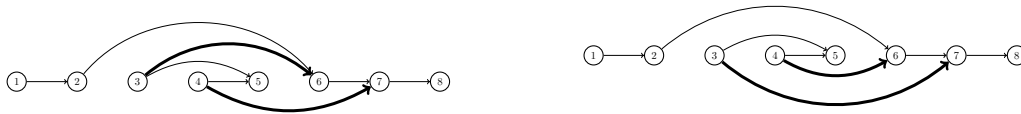


FIGURE 9. Two possible unicyclic digraphs resulting from the iterative construction process on partitions $T = \{0, 1, 0, 0, 2, 2, 2, 1\}$ and $P = \{0, 0, 2, 1, 2\}$.

Remark 4.15. Every D which is connected and unicyclic as an undirected graph can be constructed in this manner. Let D be such a graph, with M vertices and a cycle of length N . As above, without loss of generality we assume that the vertices contained in the unique cycle are labelled consecutively, say $v + 1$ through $v + N$. For each vertex i in D , let $S_i \subset [1, i - 1]$ be the set of vertices edge-connected to i and for $i \in [v + 1, v + N]$, let $C_i \subset S_i$ correspond to those edges coming from other vertices in the cycle. Then by connectedness and unicyclicity, the sets $T = \{|S_i|\}$ and $P = \{|C_i|\}$ form partitions as in the proposition, and we can follow the construction process in the proof of Proposition 4.13 with adjacency sets S_i and C_i to reconstruct D .

Corollary 4.16. *Given the construction process described in the proof of Proposition 4.13, the resulting digraph D is invertible iff N is even or $C_i = \{i - 1\}$ for all $v + 1 < i < v + N$.*

Proof. If N is even, the resulting unicyclic digraph is bipartite, and thus invertible. The requirement that $C_i = \{i - 1\}$ for all $v + 1 < i < v + N$ forces $C_{v+N} = \{v + 1, v + N - 1\}$, and is equivalent to saying the undirected cycle subgraph D' induced by vertices $\{v + 1, \dots, v + N\}$ must contain only one source and one sink vertex (i.e., $k = 1$ in the language of Theorem 3.22), and that these two vertices must be adjacent. Thus, the result follows directly from Theorem 3.22. \square

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