Encoding graphs by words and morphisms

KITTITAT IAMTHONG

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Doctoral Thesis Strathclyde Combinatorics Research Group Department of Mathematics and Statistics University of Strathclyde, Glasgow, UK Advisor: Sergey Kitaev

Disclaimer

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Chapter 2 is based on [Iam21], and it is a result of the author's original work and is the sole work of the author. Chapter 3 is based on [IK21], and it is a result of author's work in collaboration with Sergey Kitaev. Finally, Chapter 4 is based on [IJK21], and it is a result of author's work in collaboration with Ji-Hwan Jung and Sergey Kitaev.

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Abstract

This thesis is related to encoding graphs by words, where we deal with so called word-representation of graphs, relevant to them semi-transitive orientations, and more exotic ways to represent graphs via bijections with certain words and patternavoiding permutations.

In Chapter 2, we introduce a way to define classes of split graphs via iterations of morphisms and present a number of general results on word-representation of such graphs. A particular result obtained by us that goes beyond the study of split graphs, is a characterization of word-representable graphs in terms of permutations of columns of the adjacency matrices. We also provide a complete classification of word-representable split graphs defined by iteration of morphisms using two 2×2 matrices.

In Chapter 3, we study families of directed split graphs obtained by iterations of morphisms applied to the adjacency matrices and giving as the limit infinite directed split graphs. For each of such a family we ask the question on whether all graphs in the family are oriented semi-transitively (i.e. are semi-transitive) or a finite iteration k of the morphism produces a non-semi-transitive orientation (which will stay non-semi-transitive for all iterations > k). We fully classify semitransitive infinite directed split graphs in question.

In Chapter 4, we present encoding p-Riordan graphs by p-Riordan words, and encoding Riordan graphs by pattern-avoiding permutations. Also, we encode oriented Riordan graphs by balanced words over the alphabet $\{0, 1, 2\}$, and provide, as a bi-product, a proof of a known enumerative result about closed walks in the 3-cube.

This thesis is based on the papers [Iam21, IK21, IJK21].

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Chapter 1

Introduction

There are many ways to encode graphs that can be found in the literature, e.g. using the adjacency matrix, incident matrix, words, etc. The adjacency matrix is a natural option for representing a graph and it is often used to store graphs in computer memory. However, to solve efficiently certain problems we may recruit other ways to represent graphs. A suitable example of such a situation is the classical Snake-in-the-Box problem. The problem is in determining the length of a longest cycle without chords, which is called a snake, in an n-cube. In [Evd69], Evdokimov has used an encoding of paths in n-cube by words to find the asymptotic for the length. The basic idea here is that we can transfer a problem on graphs to words via an appropriate encoding and solve the problem on words, then returning the solution for the problem on graphs.

Encoding graphs by words is the main focus of this work. In the thesis, we deal with so called word-representation of graphs, relevant to them semi-transitive orientations, and more exotic ways to represent graphs via bijections with certain words and pattern-avoiding permutations. This thesis is based on the papers [Iam21, IK21, IJK21]. We begin with some background necessary to follow the

material in the thesis.

1.1 Basic Definitions in Graph Theory

We start with basic definitions in Graph Theory. In this thesis, we work with graphs having no loops or multiple edges meaning, respectively, no edges connecting the same vertex and at most one edge connecting two vertices. This type of graphs is known as *simple graphs*.

Definition 1. A (simple) graph is an ordered pair G = (V(G), E(G)), where V(G)is a set whose elements are called vertices, and E(G) is a set of paired vertices, whose elements are called edges. If $u, v \in E(G)$, we say that u and v are adjacent, or u is adjacent to v.

From the definition, a graph is defined by an ordered pair of sets, which is not always convenient to deal with. Graphs are normally represented by drawing points (vertices) and lines (edges) connecting points. For example, if $V = \{1, 2, 3, 4\}$ and $E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{3, 4\}\}$, then the graph G = (V, E) can be represented as in Figure 1.1.



Figure 1.1: Representation of a graph G = (V, E) where $V = \{1, 2, 3, 4\}$ and $E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{3, 4\}\}$

Another effective graph representation is listing all vertices and edges of a graph. Moreover, it is very common to represent a graph by a matrix, for example,

for storing the graph in computer memory.

Definition 2. Let G = (V, E) be a graph with $V = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix of G, written by $A(G) = [a_{ij}]$, is the binary n-by-n matrix in which entry a_{ij} is 1 if $\{v_i, v_j\}$ is an edge in G, and a_{ij} is 0 otherwise.

We can see that the graph in Figure 1.1 can be represented by the adjacency matrix

$$A(G) = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Note that any adjacency matrix is symmetric $(a_{ij} = a_{ji} \text{ for all } i, j)$ and the entries on the diagonal are always 0.

Definition 3. A graph H is a subgraph of a graph G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. We then write $H \subseteq G$ and say that "G contains H as a subgraph". A graph I is an induced subgraph of a graph G if $V(I) \subseteq V(G)$ and for any $u, v \in V(I), \{u, v\} \in E(I)$ if and only if $\{u, v\} \in E(G)$.

In other words, we can say that an induced subgraph is a subgraph obtained by deleting some vertices and the edges connected to them. A graph G is *complete* if every two distinct vertices are adjacent. The next definition introduces important types of induced subgraphs.

Definition 4. A clique of graph G is an induced subgraph of G that is complete. An independent set in a graph is a set of pairwise nonadjacent vertices in the graph. **Definition 5.** A directed graph or oriented graph is an ordered pair G = (V(G), E(G)), where V(G) is a set of vertices, and E(G) is a set of ordered pairs of vertices, whose elements are called (directed) edges. The first vertex of an ordered pair is tail of the edge, and the second is the head.

Similarly to ordinary graphs, in this thesis, we do not allow directed graphs to have loops (edges having the same head and tail) and multiple edges (more than one edge between a pair of vertices).

1.2 Word-representation of graphs

The main focus of Chapter 2 is on the class of graphs called *word-representable* graphs. There is a long line of research on word-representable graphs in the literature, for example, see [AKM15, BZ19, CKKP19, CKK19, CKL17, GKP18, GKZ17, Kit17]. Word-representable graphs are important as they generalize several well-known and well-studied classes of graphs such as 3-colorable graphs, comparability graphs and circle graphs [KL15]. The letters x and y alternate in a word w if removing the copies of letters different from x and y in w yields a word $xyxy \cdots$ or $yxyx \cdots$, of even or odd length. Then we can define a word-representable graph as follow.

Definition 6. A graph G = (V, E) is word-representable if there exist a word w over the alphabet V such that distinct letters x and y alternate in w if and only if $xy \in E$. We say that w represents G and w is a word-representant.

Note that any labelling of a graph is equivalent to any other labelling because letters in w can always be renamed. So, Definition 6 is valid for both labelled and unlabelled graphs. For example, the 5 vertices graphs in Figure 1.2 can be represented by the word 121342535. Thus, the graphs in Figure 1.2 are word-representable. For another example, the cycle graph on four vertices labelled 1, 2, 3, 4 in clockwise(or counterclockwise) direction is word-representable because it can be represented by the word 14213243.



Figure 1.2: The unlabelled and labelled graphs are representable by the word 121342535.

Each word-representable graph has more than one word-representant. For instance, 352513124, which is a cyclic shift of 131243525, is also a word-representant for the graphs in Figure 1.2. A word-representable graph can have a wordrepresentant which is not a cyclic shift of another word-representant. For example, the one edge graph represented by 121 is not represented by 211 or 112. The complete graph K_n of order n can be represented by 1234 or 12341234 or any permutation over $\{1, 2, ..., n\}$. The empty graph of order k can be represented by $123 \cdots kk(k-1) \cdots 1$ or $1122 \cdots kk$.

If a graph G is word-representable by a word w, then G-v can be represented by the word obtained by removing all v in w. Then, the class of word-representable graphs is hereditary, that is, removing a vertex in a word-representable graph results in a word-representable graph.

Not all graphs are word-representable. The wheel graph W_5 is the smallest (by the number of vertices) counter example as no word can represent W_5 [KP08]. A graph is *non-word-representable* if it is not word-representable. Since the class of word-representable graphs is hereditary, we also know that all graphs containing W_5 as an induced subgraph are non-word-representable. In general, it is a natural research direction to look for a characterization of word-representable graphs. We do have such a characterization in terms of semi-transitive orientations discussed in the next section, but finding other characterizations, e.g. in terms of forbidden subgraphs, is an open problem.

1.3 Semi-transitive orientations

An orientation of a directed graph is *transitive* if presence of edges $u \to v$ and $v \to z$ implies presence of the edge $u \to z$. The next definition is a generalization of the notion of a transitive orientation.

Definition 7. An orientation of a graph G = (V, E) is semi-transitive if it is acyclic and for any directed path $v_1 \rightarrow v_2 \rightarrow \cdots \rightarrow v_k$ with $v_i \in V$ for all $i \in \{1, 2, \ldots, k\}$ either

- 1. there is no edge $v_1 \rightarrow v_k$, or
- the edge v₁ → v_k is present and there are edges v_i → v_j for all 1 ≤ i ≤ j ≤ k. In other words, in this case, the (acyclic) subgraph induced by the vertices v₁, v₂,..., v_k is transitive.

A graph G = (V, E) is semi-transitive if it admits a semi-transitive orientation.

A graph obtained by changing the direction of one edge of a directed cycle is called a *semi-cycle*. A *shortcut* is a directed acyclic graph such that it is induced by the vertices of a semi-cycle and contains a pair of non-adjacent vertices. Thus, a shortcut is a directed graph satisfying the following properties:



Figure 1.3: A semi-transitive orientation of the graph in Figure 1.2.

- it is acyclic (there is no directed cycles);
- it contains at least four vertices;
- it has exactly one *source* (no edges coming in), exactly one *sink* (no edges coming out), and a directed path from the source to the sink that goes through each vertex in the graph;
- it has an edge connecting the source to the sink;
- it is not transitive.

We have an alternative definition of a semi-transitive orientation in terms of induced subgraphs.

Definition 8. An orientation of a graph is semi-transitive, if it is acyclic and contains no shortcuts.

The following theorem provides a characterization of word-representable graphs in terms of orientations.

Theorem 9 ([HKP16]). A graph is word-representable if and only if it admits a semi-transitive orientation.

Theorem 9 is very useful as we can recognise a word-representable graph by assigning to it a semi-transitive orientation. For example, we know that a graph in Figure 1.2 is word-representable because it admits a semi-transitive orientation presented in Figure 1.3.

The following simple lemma will also be of use to us in this thesis.

Lemma 10 ([KLMW]). Let K_m be a clique in a graph G. Then any acyclic orientation of G induces a transitive orientation on K_m (where the presence of edges $u \to v$ and $v \to z$ implies the presence of the edge $u \to z$). In particular, any semi-transitive orientation of G induces a transitive orientation on K_m . In either case, the orientation induced on K_m contains a single source and a single sink.

1.4 Split graphs

A *split graph* is a graph in which the vertices can be partitioned into a clique and an independent set [FH]. The paper [KLMW] initiated a systematic study of word-representability of split graphs, which was extended in a follow up paper [CKS20]. In particular, characterizations of word-representable split graphs in terms of forbidden induced subgraphs were obtained in [KLMW] and [CKS20] for cliques of sizes 4 and 5, respectively. Also, a characterization of semi-transitive orientations of split graphs was obtained in [KLMW] (see below), and split graphs were used to solve a long standing problem in the theory of word-representation in [CKS20]. We note though that currently a complete characterization of split graphs (e.g. in terms of forbidden subgraphs) seems to be a non-feasible problem, so a natural research direction is in understanding (non-)word-representable subclasses



Figure 1.4: Three types of vertices in E_{n-m} in a semi-transitive orientation of (E_{n-m}, K_m) . The vertical oriented paths are a schematic way to represent (parts of) \vec{P}

of split graphs.

Let $S_n = (E_{n-m}, K_m)$ be a word-representable split graph, where K_m is the maximal clique by the number of vertices, and E_{n-m} is the independent set. Then, by Theorem 9, S_n admits a semi-transitive orientation. Further, by Lemma 10 we know that any such orientation induces a transitive orientation on K_m with the longest directed path \vec{P} . Theorem 13 below characterizes semi-transitive orientation transitive orientation orientation.

Theorem 11 ([KLMW]). Any semi-transitive orientation of a split graph $S_n = (E_{n-m}, K_m)$ subdivides the set of all vertices in E_{n-m} into three, possibly empty, groups corresponding to each of the following types (also shown schematically in Figure 1.4), where $\vec{P} = p_1 \rightarrow \cdots \rightarrow p_m$ is the longest directed path in K_m :

- A vertex in E_{n-m} is of type A if it is a source and is connected to all vertices in {p_i, p_{i+1},..., p_j} for some 1 ≤ i ≤ j ≤ m;
- A vertex in E_{n-m} is of type B if it is a sink and is connected to all vertices in {p_i, p_{i+1},..., p_j} for some 1 ≤ i ≤ j ≤ m;

• A vertex $v \in E_{n-m}$ is of type C if there is an edge $x \to v$ for each $x \in I_v = \{p_1, p_2, \dots, p_i\}$ and there is an edge $v \to y$ for each $y \in O_v = \{p_j, p_{j+1}, \dots, p_m\}$ for some $1 \le i < j \le m$.

There are additional restrictions, given by the next theorem, on relative positions of the neighbours of vertices of types A, B and C.

Theorem 12 ([KLMW]). Let $S_n = (E_{n-m}, K_m)$ be oriented semi-transitively with $\vec{P} = p_1 \rightarrow \cdots \rightarrow p_m$. For a vertex $x \in E_{n-m}$ of type C, there is no vertex $y \in E_{n-m}$ of type A or B, which is connected to both $p_{|I_x|}$ and $p_{m-|O_x|+1}$. Also, there is no vertex $y \in E_{n-m}$ of type C such that either I_y , or O_y contains both $p_{|I_x|}$ and $p_{m-|O_x|+1}$.

One can now classify semi-transitive orientations on split graphs.

Theorem 13 ([KLMW]). An orientation of a split graph $S_n = (E_{n-m}, K_m)$ is semi-transitive if and only if

- (i) K_m is oriented transitively;
- (ii) each vertex in E_{n-m} is of one of the three types in Theorem 11;
- (iii) the restrictions in Theorem 12 are satisfied.

1.5 Morphisms

Let A and B be alphabets (possibly A = B). A map $\varphi : A^* \to B^*$ is called a morphism, if we have $\varphi(uv) = \varphi(u)\varphi(v)$ for any $u, v \in A^*$. A morphism φ can be defined by defining $\varphi(a)$ for each $a \in A$. A particular property of a morphism φ is that $\varphi(\varepsilon) = \varepsilon$, where ε is the empty word. For example, Thue-Morse squence t_0, t_1, t_2, \ldots is a well-known sequence of words defined by iteration of morphism. It starts with $t_0 = 0$ and $t_i = \theta(t_{i-1})$ where $i \ge 1$ and $\theta : \{0, 1\} \to \{0, 1\}^2$ is a morphism defined by $\theta(0) = 01$ and $\theta(1) = 10$. The first few initial iterations of t_0, t_1, t_2, \ldots are

$0, 01, 0110, 01101001, 0110100110010110, \ldots$

Morphisms are a central object in the area of combinatorics on words [Lot83], and there is a natural extension of the notion to two, or more, dimensions. Indeed, one can begin with a matrix M whose entries are elements of A, and then obtain $\varphi(M)$ by substituting each element in M by matrices having the same dimensions and given by some substitution rules. For instance, we define a sequence of binary matrices S_0, S_1, S_2, \ldots by $S_0 = [1]$ and $S_i = \phi(S_{i-1})$ where $i \ge 1$ and ϕ is a morphism defined by $0 \mapsto \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$ and $1 \mapsto \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$. The first four iterations of this 2-dimensional morphism are

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

where the lower triangular matrices define a well-known shape, Sierpinski triangle.

Relevance of (2-dimensional) morphisms to split graphs is coming from the ideas communicated in [CKKK19], where patterns in adjacency matrices are considered to study word-representability of graphs, and the notion of an infinite word-representable graph is introduced in Sections 2.2 and 3.2.

1.6 Patterns in permutations

We consider permutations in the one-line notation, and a permutation of length n is called an *n*-permutation. The reduce form of a permutation π is the permutation $\operatorname{red}(\pi)$ obtained from π by substituting the *i*-th smallest element by *i*. For example, $\operatorname{red}(4287)=2143$.

Let $\tau = \tau_1 \tau_2 \cdots \tau_k$ and $\pi = \pi_1 \pi_2 \cdots \pi_n$ be permutations such that $k \leq n$. We say that the pattern τ occurs in the permutation π if there are indices $1 \leq i_1 < i_2 < \cdots < i_k \leq n$ such that $\operatorname{red}(\pi_{i_1} \pi_{i_2} \cdots \pi_{i_k}) = \tau$. Moreover, a permutation π avoids a pattern τ if there is no occurrence of τ in π . For example, the permutation 14235 has five occurrence of the pattern 123, namely, the subsequences 145, 123, 125, 135 and 235, while the permutation 34512 avoids the pattern 132 (has no occurrences of it). Permutation patterns have been the subject of extensive research in the literature [Kit11].

A well-known result [Kit11, Table 6.1], to be used in this thesis, states that the number of *n*-permutations that avoid simultaneously the patterns 123 and 132 is 2^{n-1} . This can be proved using a bijection ψ from the set of binary words of length n-1 to the set of restricted *n*-permutations that is denoted by $S_n(123, 132)$. Think of constructing a permutation in $S_n(123, 132)$ by inserting elements $1, 2, \ldots, n$ one by one, starting from 1 and continuing with the least available element, into n empty slots and observing that at each step an element i can only be inserted in one of the two rightmost empty slots to avoid the patterns 123 and 132; the element n will be inserted in a unique way. Thus, given a binary word $b_1b_2\cdots b_{n-1}$,

 ψ uses the process of insertion, and places the element *i* to the left (resp., right) available slot if $b_i = 0$ (resp., 1). For example, $\psi(011001) = 7546312$.

1.7 Riordan graphs and *p*-Riordan graphs

Riordan graphs were introduced in [CJKM19a, CJKM19b] and they are a farreaching generalization of the well-known and well studied Pascal graphs and Toeplitz graphs, and also some other families of graphs. The Riordan graphs are proved to have a number of interesting (fractal) properties [CJKM19a], and spectral properties of Riordan graphs were studied in [CJKM19b].

Riordan graphs

Definition 14. Let $L = [l_{ij}]_{i,j\geq 0}$ be an infinite matrix over integral domain κ . If there exists a pair of generating functions $(g, f) \in \kappa[[t]] \times \kappa[[t]], f(0) = 0$ such that

$$gf^j = \sum_{i \ge 0} l_{ij}t^i, j \ge 0$$
 or equivalently $l_{ij} = [t^i]gf^j$

then the matrix L is called a Riordan Matrix (or, a Riordan array) over κ generated by g and f.

In other words, we can say that a Riordan matrix $L = [\ell_{ij}]_{i,j\geq 0}$ generated by two formal power series $g = \sum_{n=0}^{\infty} g_n t^n$ and $f = \sum_{n=1}^{\infty} f_n t^n$ in $\mathbb{Z}[[t]]$ is denoted as (g, f) and defined as an infinite lower triangular matrix whose *j*-th column generating function is gf^j , i.e. $\ell_{ij} = [t^i]gf^j$ where $[t^k] \sum_{n\geq 0} a_n t^n = a_k$. Usually, we write L = (g(t), f(t)) or (g, f) for a Riordan Matrix generated by g and f. Note that (g, f) is invertible if and only if $g_0 \neq 0$ and $f_1 \neq 0$, in which case (g, f) is called *proper*. A simple graph G of order n is said to be a *Riordan graph* if the adjacency matrix A(G) can be expressed as

$$A(G) \equiv (tg, f)_n + (tg, f)_n^T \pmod{2} \tag{1.1}$$

for some generating functions g and f over \mathbb{Z} where $(tg, f)_n$ is the $n \times n$ leading principle matrix of the Riordan matrix (tg, f). A Riordan graph G on n vertices with the adjacency matrix A(G) given by equation (1.1) is denoted as $G = G_n(g, f)$. If we let $A(G) = (a_{i,j})_{1 \le i,j \le n}$, then, for $i \ge j$,

$$a_{i,j} = a_{j,i} \equiv [t^{i-2}]gf^{j-1} \pmod{2}.$$

In particular, if $[t^0]g \equiv [t^1]f \equiv 1 \pmod{2}$, then the graph $G_n(g, f)$ is called *proper*. We denote the set of Riordan graphs with n vertices by \mathcal{RG}_n . When defining Riordan graphs we assume, without loss the generality, that g and f have binary coefficients. Then, the number r_n of Riordan graphs of order $n \geq 1$ is known from [CJKM19a] to be

$$r_n = \frac{4^{n-1} + 2}{3}.\tag{1.2}$$

Example 15. Let $g = \frac{1}{1-t}$ and $f = \frac{t}{1-t}$, then

$$gf^{j} = \frac{1}{1-t} \left(\frac{t}{1-t}\right)^{j} = \frac{t^{j}}{(1-t)^{j+1}} = \sum_{i=0}^{\infty} \binom{i}{j} t^{i}, j \ge 0.$$

So, the Riordan matrix (g, f) is

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & \cdots \\ 1 & 1 & 0 & 0 & 0 & \cdots \\ 1 & 2 & 1 & 0 & 0 & \cdots \\ 1 & 3 & 3 & 1 & 0 & \cdots \\ 1 & 4 & 6 & 4 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

which is an infinite lower triangular matrix with properties analogous to the Pascal triangle. Then, the adjacency matrix of $G_6(g, f)$ is

0	1	1	1	1	1
1	0	1	0	1	0
1	1	0	1	1	0
1	0	1	0	1	0
1	1	1	1	0	1
1	0	0	0	1	0

and the graph $G_6(g, f)$ is shown in Figure 1.5.



Figure 1.5: The graph $G_6(g, f)$ in Example 15

There are several naturally defined classes/families of Riordan graphs [CJKM19a, CJKM19b]. A Riordan graph $G_n(g,t)$ is said to be of the *Appell type*. Riordan graphs of the Appell type are also known as *Toeplitz graphs*. Toeplitz graphs have been studied in [CJKM19a, vDTT⁺96, NP14]. A Riordan graph $G_n(g,tg)$ is said to be of the *Bell type* and it has been studied in [CJKM19a, Juna]. The well-known *Pascal graph* $G_n\left(\frac{1}{1-t}, \frac{t}{1-t}\right)$ is a particular example of a Bell type Riordan graph, and it is the only such graph of type (1 + f, f), also considered in this thesis. Finally, a Riordan graph $G_n(f', f)$ is said to be of the *derivative type* and it has been studied in [CJKM19a].

Oriented Riordan graphs and *p*-Riordan graphs.

There is a natural generalization of the notion of a Riordan graph that was introduced in [Junb]. This notion is obtained by replacing "mod 2" by "mod p" in the definition of a Riordan graph. While the definition makes sense for any integer $p \ge 2$, it is normally assumed that p is a prime number to resolve the invertibility issues preventing us from being able to analyze such graphs. In particular, the number $r_n^{(p)}$ of p-Riordan graphs for a prime p was derived in [Junb], and it is given by

$$r_n^{(p)} = \frac{p^{2(n-1)} + p}{p+1},\tag{1.3}$$

while no enumeration is known for a non-prime p. Setting p = 2 in (1.3) we recover the number of Riordan graphs given by (1.2), while setting p = 3 in (1.3) we obtain the number \tilde{r}_n of oriented Riordan graphs of order n:

$$\tilde{r}_n = \frac{3^{2(n-1)} + 3}{4}.$$
(1.4)

For $p \geq 3$, p-Riordan graphs can be thought of as weighted Riordan graphs.

In the case of a *p*-Riordan graph *G*, in some contexts it is convenient to let the elements of the adjacency matrix A(G) be coming from the set $\{\lfloor p/2 \rfloor, \ldots, -1, 0, 1, \ldots, \lfloor p/2 \rfloor\}$. However, in this thesis, it is more convenient to let these elements be in the set $\{0, 1, \ldots, p-1\}$. In particular, oriented Riordan graphs have adjacency matrices' elements in $\{0, 1, 2\}$. We denote the set of *p*-Riordan graphs with *n* vertices by $\mathcal{RG}_n^{(p)}$.

1.8 Organisation of this thesis

Up to this point, we have already provided a comprehensive overview of basic notions to be used in the thesis. In Chapter 2, we first give a characterization of word-representable split graphs in terms of permutations of columns of the adjacency matrices. Then, we focus on the study of word-representability of split graphs obtained by iterations of a morphism, a notion coming from combinatorics on words. We prove a number of general theorems and provide a complete classification in the case of morphisms defined by 2×2 matrices.

After that, in Chapter 3, we study semi-transitivity of families of directed split graphs obtained by iterations of morphisms applied to the adjacency matrices and giving in the limit infinite directed split graphs. We fully classify semi-transitive infinite directed split graphs when a morphism in question can involve any $n \times m$ matrices over $\{-1, 0, 1\}$ with a single natural condition.

Finally, in Chapter 4, we introduce the notion of a p-Riordan word, and show how to encode p-Riordan graphs by p-Riordan words. For special important cases of Riordan graphs (the case p = 2) and oriented Riordan graphs (the case p = 3) we provide alternative encodings in terms of pattern-avoiding permutations and certain balanced words, respectively. As a bi-product of our studies, we provide an alternative proof of a known enumerative result on closed walks in the cube.

Part I

Encoding Split Graphs Generated by Morphisms

Chapter 2

Word-representability of Split Graphs Generated by Morphisms

In this chapter, based on [Iam21], we introduce a way to define adjacency matrices of split graphs in term of any binary matrices, and provide some results on wordrepresentability of split graphs. We also present a number of general results on split graphs generated by morphisms in Section 2.2. After that, in Section 2.3, we provide a complete classification of word-representable split graphs defined by iteration of morphisms using two 2×2 matrices (the results in this section are summarized in Tables 2.1 and 2.2).

2.1 Adjacency matrices of split graphs and general results

Definition 16. Let M be a binary $m \times n$ matrix. Define S(M) to be the matrix

$$\left[\begin{array}{cc} L_n & M^T \\ M & O_m \end{array}\right]$$

where O_m is the $m \times m$ zero matrix and L_n is the $n \times n$ matrix such that all diagonal entries are 0's and all other entries are 1's.

It is easy to see that for any binary $m \times n$ matrix M, S(M) is the adjacency matrix of a split graph with the maximal clique of order n or n+1. We denote the split graph by G(M). Clearly, M gives edges between the clique and independent set in G(M), and the order of the maximal clique depends on the existence of a $11 \cdots 1$ row in M.

Example 17. If
$$M = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$
 then
$$S(M) = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$



Figure 2.1: The split graph G(M) given by S(M) in Example 17.

is the adjacency matrix of the graph shown in Figure 2.1.

Remark 18. If M is a zero matrix, then G(M) is a disjoint union of a clique and isolated vertices and is word-representable, because the clique is semi-transitively (in fact, transitively) orientable and there are no other edges in G(M).

The following lemma is Lemma 8 in [KLMW].

Lemma 19 ([KLMW]). Let $S_n = (E_{n-m}, K_m)$ be a split graph with the maximum clique K_m , and a spit graph S_{n+1} is obtained from S_n by either adding a vertex of degree 0 (to E_{n-m}), or adding a vertex of degree 1 (to E_{n-m}), or by "copying" a vertex (either in E_{n-m} or in K_m), that is, by adding a vertex whose neighbourhood is identical to the neighbourhood of a vertex in S_n . Then S_n is word-representable if and only if S_{n+1} is word-representable.

To analyze word-representability of a given split graph, by Lemma 19 we can delete vertices of degree 0 and vertices of degree 1, as well as delete all but one vertex having the same neighborhood.

Proposition 20. Let M be an $m \times n$ matrix. If every row, or every column of M is of the form $00 \cdots 0$ or $11 \cdots 1$, then G(M) is word-representable.

Proof. If every row of M consists of all 0's or all 1's then in G(M), each vertex in the independent set is an isolated vertex, or is connected to every vertex in

the clique. By Lemma 19, word-representability of G(M) is equivalent to wordrepresentability of either the clique K_{n+1} , or the disjoint union of a clique (K_n or K_{n+1}) and an isolated vertex, which are clearly semi-transitively orientable, and thus, by Theorem 9, word-representable.

On the other hand, if every column of M consists of all 0's or all 1's then the neighborhood of each vertex in the independent set is the same and, by Lemma 19, word-representability of G(M) is equivalent to word-representability of the clique K_n with a vertex x connected to some, maybe none or all of clique's vertices. If w.l.o.g. x is connected to vertices $1, 2, \ldots, p, 0 \le p \le n$, in K_n formed by the vertices $1, 2, \ldots, n$, then the word $x12 \cdots px(p+1)(p+2) \cdots n$ represents the graph.

It is obvious that if M^* is a matrix obtained by a row or column permutation of a matrix M, then $G(M^*)$ is a split graph obtained by relabelling the vertices of the graph G(M). Hence we get the following lemma.

Lemma 21. Let M be an $m \times n$ binary matrix and M^* is a matrix obtained from a sequence of row and/or column permutations of M. Then, G(M) is wordrepresentable if and only if $G(M^*)$ is word-representable.

For any $m \times n$ binary matrix M, we can consider the n columns of M as connectivity of the vertices in the maximal clique (first n rows/columns of S(M)) and m rows of M as connectivity of the vertices in the independent set (last mrows/columns of S(m)). However, we note that M have the maximal clique of size n+1 if $111\cdots 1$ is a row in M. Then, we can move the vertex in the independent set which is connected to every vertex in the clique of size n to be one of the vertices in the maximal clique. So, we can create a new $(m-1) \times (n+1)$ binary matrix N such that the graphs G(M) and G(N) are the same, and every row of N is not equal to $111\cdots 1$. With this idea in mind, we obtain the following lemma.

Lemma 22. Let $M := [m_{ij}]_{m \times n}$ be an $m \times n$ binary matrix such that $m_{k1} = m_{k2} = \cdots = m_{kn} = 1$ for some $k \in \{1, 2, \ldots, m\}$. If

$$N = \begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1n} & 0 \\ m_{21} & m_{22} & \cdots & m_{2n} & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ m_{(k-1)1} & m_{(k-1)2} & \cdots & m_{(k-1)n} & 0 \\ m_{(k+1)1} & m_{(k+1)2} & \cdots & m_{(k+1)n} & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ m_{m1} & m_{m2} & \cdots & m_{mn} & 0 \end{bmatrix},$$

is an $(m-1) \times (n+1)$ binary matrix, then G(M) is isomorphic to G(N).

Proof. Let M^* be the matrix obtained from M by making the k^{th} row be the first row. That is,

$$M^* = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & & \vdots \\ m_{(k-1)1} & m_{(k-1)2} & \cdots & m_{(k-1)n} \\ m_{(k+1)1} & m_{(k+1)2} & \cdots & m_{(k+1)n} \\ \vdots & \vdots & & \vdots \\ m_{m1} & m_{m2} & \cdots & m_{mn} \end{bmatrix}$$

Since M^* is obtained by reordering rows of M, $G(M^*)$ is obtained by relabeling the vertices of G(M), and thus $G(M^*)$ is isomorphic to G(M). Note that $S(M^*) =$



Figure 2.2: Non-word-representable split graphs T_1, T_2, T_3, T_4 .

S(N), and so $G(M^*)$ and G(N) are the same graph. Hence G(M) is isomorphic to G(N).

It is known [Kit17] that there are no non-word-representable graphs of order less than 6 and the only non-word-representable graph on 6 vertices is the wheel graph W_5 , which is not a split graph. Thus, G(M) is word-representable if M is an $m \times n$ matrix and $m + n \leq 6$. In [KLMW], it is shown that any split graph S with maximum clique K_4 is word-representable if and only if S does not contain the graphs T_1 , T_2 , T_3 and T_4 shown in Figure 2.2 as induced subgraphs. As a corollary to this result, we have the following theorem.

Theorem 23. Let A be an $m \times 4$ binary matrix without all 1's rows. Then, G(A)is word-representable if and only if the rows and columns of A cannot be permuted

	г			г		г			-	1	г			٦		1	1	1	0
	1	1	0	0		1	1	0	0		1	0	1	1		1	1	0	
to be a matrix containing	1	0	1	0		1	0	1	0		1	1	0	1	or	1	T	0	
					l ′		-									1	0	0	1
	Γ_0	1	1	0		L^1	0	0	1	i -	L^1	1	1 0	0		1	Ο	1	1
as a submatrix																L	0	T	Γ

a submatrix.

Let x^n denotes $xx \cdots x$ where x is repeated n times. The next theorem gives a sufficient condition for word-representability of a given graph G(M).

Theorem 24. Let M be an $m \times n$ binary matrix. If there is a sequence of column permutations of M giving the matrix such that each row of M is of the form $0^r 1^s 0^t$ for some non-negative integers r, s, t, then G(M) is word-representable.

Proof. Assume that M^* is the matrix obtained from a sequence of column permutations of M and each row of M^* is of the form $0^r 1^s 0^t$ where r, s, t are non-negative integers. Let the i^{th} row/column of the adjacency matrix $S(M^*)$ correspond to vertex i in $G(M^*)$. So the clique C in $G(M^*)$ contains vertices $1, 2, \ldots, n$ and the independent set I in $G(M^*)$ contains vertices $n + 1, n + 2, \ldots, n + m$. Assign the orientation of edges in $G(M^*)$ as $i \to j$ if and only if i < j. We have that $1 \to 2 \to \cdots \to n$ is the longest path in the transitively oriented C, and the edges between C and I are oriented from C to I. Thus, each edge in the independent set is of type B, and we are done by Theorems 9 and 13.

We have the following important generalization of Theorem 24.

Theorem 25. Let M be an $m \times n$ binary matrix without all 1's rows. The split graph G(M) is word-representable if and only if M satisfies the following conditions:

- (i) there is a sequence of column permutations of M giving a matrix M* where every row is of the form 0^r1^s0^t or 1^r0^s1^t for some nonnegative integers r, s, t, and
- (ii) for any row of M* of the form 1^a0^b1^c for some positive integers a, b, c, there is no other row having 1's in all positions from a to a + b + 1.

Proof. " \Leftarrow ." Assign the orientation of edges in $G(M^*)$ as $i \to j$ if i < j except if j > n (i.e. j is a vertex in the independent set) and the row in M^* corresponding

to j is of the form $1^r 0^s 1^t$, in which case we still orient $i \to j$ for $1 \le i \le r$ but $j \to i$ for $r + s + 1 \le i \le n$. The vertices in the independent set will then be of types B and C, and taking into account condition (ii), Theorems 9 and 13 can be applied to see that $G(M^*)$ is word-representable, and thus G(M) is word-representable by Lemma 21.

" \Rightarrow ." By Theorem 9, G(M) admits a semi-transitive orientation. By Theorem 13, under this orientation the clique is oriented transitively, and we can rename the vertices of the clique, if necessary so that the longest path would be formed by $1 \rightarrow 2 \rightarrow \cdots \rightarrow n$. Note that renaming vertices in the clique corresponds to permuting columns in M giving M^* . But then, conditions (ii) and (iii) in Theorem 13 give conditions (i) and (ii) in this theorem.

Remark 26. If M has an all 1's row, we can see that Theorems 23 and 25 cannot be applied. However, we can use Theorem 22 to change M into an $(m-1) \times (n+1)$ matrix N which does not contain all 1's row. So we can apply the theorems to matrix N instead of M because G(N) is isomorphic to G(M). This observation also applies to Corollary 33 below.

We can see that Theorem 25 allows us to answer the question on word-representability of G(M) by looking at permutations of columns in M. Let $M = [m_{ij}]_{m \times n}$ be an $m \times n$ matrix and $\rho = \rho_1 \rho_2 \cdots \rho_n$ is a permutation of $\{1, 2, \dots, n\}$ written in one-line notation. We say that

$$M^{*} = \begin{bmatrix} m_{1\rho_{1}} & m_{1\rho_{2}} & \cdots & m_{1\rho_{n}} \\ m_{2\rho_{1}} & m_{2\rho_{2}} & \cdots & m_{2\rho_{n}} \\ \vdots & \vdots & \ddots & \vdots \\ m_{m\rho_{1}} & m_{m\rho_{2}} & \cdots & m_{m\rho_{n}} \end{bmatrix}$$

is the matrix obtained from reordering columns of M in the order given by ρ . The key approach given by Theorem 25 is finding a permutation ρ that turns each row of M^* into the form $0^r 1^s 0^t$ or $1^r 0^s 1^t$ (so, all 1's in M^* are cyclically consecutive). Interestingly, to prove word-representability results in this chapter, only rows of the form $0^r 1^s 0^t$ are used, so that condition (ii) in Theorem 25 is not applicable.

Example 27. In the matrix
$$M = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

we can ignore rows 2, 4, 6 and 8 because all entries in these rows are zero. Then we need to find a permutation $\rho = \rho_1 \rho_2 \cdots \rho_8$ making

- columns 1, 4, 6 and 7 be (cyclically) consecutive in rows 1;
- columns 1, 3, 5 and 7 be (cyclically) consecutive in row 3 and 7;
- columns 2, 3, 6 and 7 be (cyclically) consecutive in row 5.

It can be implied from the first and the second bullet points that 1 and 7 must be consecutive in ρ and then, w.l.o.g., 4 and 6 are next to the left of these numbers and 3 and 5 are next to the right of them (cyclically). Hence ρ contains

$$\{4,6\},\{1,7\},\{3,5\}$$

where numbers in $\{\}$ are consecutive in ρ but are in some unknown to us order. But then, we get a contradiction with the second bullet point. Hence, there is no such ρ and G(M) is non-word-representable by Theorem 25.

2.2 General results on split graphs generated by morphisms

In this section, we discuss rather general results on split graphs generated by morphisms, thus preparing ourselves for a classification of the case of 2×2 matrices coming in the next section.

Definition 28. Let A, B be $m \times n$ binary matrices. The matrix $M^k(A, B)$ is said to be the k^{th} -iteration of the 2-dimensional morphism applied to the 1×1 matrix [0] which maps [0] $\rightarrow A$ and [1] $\rightarrow B$. Moreover, we write $S^k(A, B)$ for the matrix $S(M^k(A, B))$ and $G^k(A, B)$ for the graph with the adjacency matrix $S^k(A, B)$.

Example 29. Let
$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$
 and $B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Then we have

$$M^{0}(A,B) = \begin{bmatrix} 0 \end{bmatrix}, \quad M^{1}(A,B) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad M^{2}(A,B) = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$



Figure 2.3: The split graph $G^2(A, B)$ corresponding to the adjacency matrix $S^2(A, B)$ in Example 29.

$$Then, S^{2}(A,B) = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} and G^{2}(A,B) is shown in Figure 2.3.$$

Remark 30. If A is a zero matrix, then $M^k(A, B)$ is always a zero matrix for any $m \times n$ matrix B and positive integer k. So, by Remark 18, $G^k(A, B)$ is word-representable.

The case of A = B

In this case, both [0] and [1] are mapped to the same matrix A, so if A is an $m \times n$ binary matrix, then

$$S^{k}(A,A) = \begin{bmatrix} L_{n^{k}} & A_{k}^{T} \\ A_{k} & O_{m^{k}} \end{bmatrix} \quad \text{where} \quad A_{k} = \underbrace{\begin{bmatrix} A & A & \cdots & A \\ A & A & \cdots & A \\ \vdots & \vdots & \ddots & \vdots \\ A & A & \cdots & A \end{bmatrix}}_{n^{k} \text{ columns}}$$

Clearly, A_k is an $n^k \times m^k$ matrix and $S^k(A, A) = S(A_k)$, so $G^k(A, A)$ is isomorphic to $G(A_k)$.

Theorem 31. Let A be an $m \times n$ binary matrix. For $k \ge 1$, $G^k(A, A)$ is word-representable if and only if G(A) is word-representable.

Proof. Firstly, we label a vertex of $G^k(A, A)$ by i if it is represented by the i^{th} column/row in $S^k(A, A)$. Note that rows $i, m+i, 2m+i, \ldots, (m^{k-1}-1)m+i$ in A_k are identical for any $i \in \{1, 2, \ldots, m\}$, and columns $j, n+j, 2n+j, \ldots, (n^{k-1}-1)n+j$ in A_k are also identical for any $j \in \{1, 2, \ldots, n\}$. So, for any $i \in \{1, 2, \ldots, m\}$, the vertices of $G^k(A, A)$ in $R_i := \{i+n^k, m+i+n^k, 2m+i+n^k, \ldots, (m^{k-1}-1)m+i+n^k\}$ have the same neighborhoods. Similarly, any two vertices of $G^k(A, A)$ in $C_j := \{j, n+j, 2n+j, \ldots, (n^{k-1}-1)n+j\}$ are connected to the same vertices in the independent set for any $j \in \{1, 2, \ldots, n\}$. Thus, by Lemma 19, $G^k(A, A)$ is word-representable if and only if the graph G obtained by deleting all vertices but the smallest one in R_i and C_j for all $i, j \in \{1, 2, \ldots, n\}$ is word-representable. But G is exactly G(A), which complete the proof.
Corollary 32. If A is an $m \times n$ binary matrix such that $m + n \leq 6$, then $G^k(A, A)$ is word-representable for any $k \geq 0$.

Proof. Since the smallest non-word-representable split graph is of order 7, all split graphs of orders less than 7 are word-representable. Hence $G^k(A, A)$ is word-representable for any $m \times n$ matrix A where $m + n \leq 6$.

Moreover, together with Theorem 23, we have the following result.

Corollary 33. Let A be an $m \times 4$ binary matrix with no all 1's row. For any integer k, the graph $G^{k}(A, A)$ is word-representable if and only if the rows and columns of A cannot be permuted to be a matrix containing $\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$, $\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix}$, $\begin{bmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}$ or $\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}$ as a submatrix.

The case of $A \neq B$

In what follows, A and B can be distinct.

Proposition 34. If every row, or every column, in $m \times n$ matrices A and B is either 0^n or 1^n , then $G^k(A, B)$ is word-representable for any $k \ge 0$.

Proof. If every row (resp., column) in A and B is either 0^n or 1^n , then every row (resp., column) in $M^k(A, B)$ is either 0^{n^k} or 1^{n^k} , so by Proposition 20, $G^k(A, B)$ is word-representable.

Theorem 35. Let A and B be $m \times n$ binary matrices. Suppose that A^* and B^* are the matrices obtained from reordering columns of A and B, respectively, in order given by a permutation $\sigma = \sigma_1 \sigma_2 \cdots \sigma_n$. Then $G^k(A, B)$ is word-representable if and only if $G^k(A^*, B^*)$ is word-representable for any $k \ge 0$.

Proof. The case k = 0 is trivial, so assume that $k \ge 1$. We claim that $M^k(A^*, B^*)$ is obtained from a permutation of columns in $M^k(A, B)$. We will prove the claim by induction on k. Note that $M^1(A, B) = A$ and $M^1(A^*, B^*) = A^*$. So $M^1(A^*, B^*)$ is the matrix obtained from reordering columns of $M^1(A, B)$. Suppose that l is a positive integer and $M^l(A^*, B^*)$ is the matrix obtained from reordering columns of $M^l(A, B)$ in order given by a permutation $\tau = \tau_1 \tau_2 \cdots \tau_{n^l}$. Let $M^l(A, B) = \begin{bmatrix} C_1 & C_2 & \cdots & C_{n^l} \end{bmatrix}$ where C_i is the i^{th} column of $M^l(A, B)$. Then $M^l(A^*, B^*) = \begin{bmatrix} C_{\tau_1} & C_{\tau_2} & \cdots & C_{\tau_{n^l}} \end{bmatrix}$. For the next iteration of morphism, each column C_i of $M^l(A, B)$ is mapped to n columns $C_{i,1}, C_{i,2}, \ldots, C_{i,n}$, and each column C_{τ_i} of $M^l(A^*, B^*)$ is mapped to n columns $C_{\tau_i,\sigma_1}, C_{\tau_i,\sigma_2}, \ldots, C_{\tau_i,\sigma_n}$. So we have

$$M^{l+1}(A,B) = \begin{bmatrix} C_{1,1} \ C_{1,2} \ \cdots \ C_{1,n} \ \cdots \ C_{n^l,1} \ C_{n^l,2} \ \cdots \ C_{n^l,n} \end{bmatrix}$$

and

$$M^{l+1}(A^*, B^*) = \begin{bmatrix} C_{\tau_1, \sigma_1} & C_{\tau_1, \sigma_2} & \cdots & C_{\tau_1, \sigma_n} & \cdots & C_{\tau_n l, \sigma_1} \\ C_{\tau_n l, \sigma_2} & \cdots & C_{\tau_n l, \sigma_n} \end{bmatrix}.$$

A group of columns $C_{i,1}, C_{i,2}, \ldots, C_{i,n}$ is called *block* B_i . Firstly, we can see that reordering the blocks $B_1, B_2, \ldots, B_{n^l}$ of $M^{l+1}(A, B)$ in order given by τ , and then reordering columns in every block B_i in order given by σ , yields the matrix $M^{l+1}(A^*, B^*)$. Thus, $M^{l+1}(A^*, B^*)$ is obtained by a column permutation of $M^{l+1}(A, B)$ and our claim is true. Hence, by Lemma 21, $G^k(A, B)$ is wordrepresentable if and only if $G^k(A^*, B^*)$ is word-representable for any positive integer k. Next theorem is a natural extension of Theorem 35 to the case of row permutations, and it can be proved in a similar way to the proof of Theorem 35, so we omit the proof.

Theorem 36. Let A and B be $m \times n$ binary matrices. Suppose that A^* and B^* are the matrices obtained from reordering rows of A and B, respectively, in order given by the same permutation. Then $G^k(A, B)$ is word-representable if and only if $G^k(A^*, B^*)$ is word-representable for any $k \ge 0$.

So, we can reorder rows and columns of given matrices A and B while preserving the word-representability of $G^k(A, B)$. If A contains at least one 0, we can reorder rows and columns of A to make the leftmost bottom entry be a 0 (the matrix B will be changed by the same permutation of rows and columns as those applied to A). Thus, in what follows, if A is not all-one matrix, w.l.o.g. we can assume that the leftmost bottom entry of A is always 0. Then, the $m \times n$ leftmost bottom submatrix of $M^2(A, B)$ is A since $M^1(A, B) = A$. Moreover, the $m^{k-1} \times n^{k-1}$ leftmost bottom submatrix of $M^k(A, B)$ is $M^{k-1}(A, B)$. Thus, the limit $\lim_{k\to\infty} M^k(A, B)$, called a fixed point of the morphism, is well-defined. So, we have that $G^i(A, B)$ is an induced subgraph of $G^k(A, B)$ if $i \leq k$ and the notion of the infinite split graph G(A, B) is well-defined in the case when A has a 0 as the leftmost bottom entry. So we are interested in the smallest integer l (possibly non-existing) that $G^l(A, B)$ is nonword-representable for given A and B (then $G^i(A, B)$ is non-word-representable for $i \geq l$).

Definition 37. Suppose that a matrix A has a 0 as the leftmost bottom entry. The index of word-representability IWR(A, B) of an infinite split graph G(A, B)is the smallest integer l such that $G^{l}(A, B)$ is non-word-representable. If such ldoes not exist, that is, if $G^{l}(A, B)$ is word-representable for all l, then $l := \infty$. If the leftmost bottom entry of A is 1 (so that the $\lim_{k\to\infty} M^k(A, B)$ may not be well-defined as the sequence of graphs $G^k(A, B)$, for $k \ge 0$, may not be a chain of induced subgraphs) then IWR(A, B) is still defined in the same way even though G(A, B) may not be defined.

Note that since $G^0(A, B)$ is a graph with one vertex, we have $IWR(A, B) \ge 1$. Even though Definition 37 is very similar to the respective definition of the index of word-representability of an infinite *Toeplitz graph* in [CKKK19] (where the index in our context would be the maximum l such that $G^l(A, B)$ is word-representable), it is more flexible as it makes sense in the situation when the leftmost bottom entry of A is 1.

Theorem 38. Let
$$A = [a_{ij}]$$
 and $B = [b_{ij}]$ be $m \times n$ binary matrices, and

$$C = \begin{bmatrix} a_{p_1q_1} & a_{p_1q_2} & \cdots & a_{p_1q_t} \\ a_{p_2q_1} & a_{p_2q_2} & \cdots & a_{p_2q_t} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p_sq_1} & a_{p_sq_2} & \cdots & a_{p_sq_t} \end{bmatrix} \text{ and } D = \begin{bmatrix} b_{p_1q_1} & b_{p_1q_2} & \cdots & b_{p_1q_t} \\ b_{p_2q_1} & b_{p_2q_2} & \cdots & b_{p_2q_t} \\ \vdots & \vdots & \ddots & \vdots \\ b_{p_sq_1} & b_{p_sq_2} & \cdots & b_{p_sq_t} \end{bmatrix}$$

be $s \times t$ submatrices of A and B, respectively, where $1 \leq p_1 < p_2 < \cdots < p_s \leq m$ and $1 \leq q_1 < q_2 < \cdots < q_t \leq n$. For any positive integer k, if $G^k(C, D)$ is non-word-representable, then $G^k(A, B)$ is non-word-representable.

Proof. First, we will prove by induction that $M^k(C, D)$ is a submatrix of $M^k(A, B)$ for any positive integer k. It is obvious that $M^1(C, D) = C$ is a submatrix of $M^1(A, B) = A$. Let l be a positive integer such that $M^l(C, D)$ is a submatrix of $M^l(A, B)$ on the columns $c_1, c_2, \ldots, c_{t^l}$ and rows $r_1, r_2, \ldots, r_{s^l}$. For the next iteration of morphism, $M^{l+1}(A, B)$ is formed by replacing each entry of $M^l(A, B)$ with either A or B. So the columns $(c_i - 1)n + q_j$ for $1 \le i \le t^l, 1 \le j \le t$, and rows $(r_i - 1)m + p_j$ for $1 \le i \le s^l$, $1 \le j \le s$, form the matrix $M^{l+1}(C, D)$. Hence $M^k(C, D)$ is a submatrix of $M^k(A, B)$ for any $k \ge 1$. Therefore, $G^k(A, B)$ contains $G^k(C, D)$ as an induced subgraph for $k \ge 1$. As the property of wordrepresentability is hereditary, we have that non-word-representability of $G^k(C, D)$ implies non-word-representability of $G^k(A, B)$.

Theorem 38 gives a useful tool to study non-word-representability of $G^k(A, B)$ for larger A and B. Indeed, a starting point to justify suspected non-wordrepresentability of $G^k(A, B)$ can be analysis of smaller submatrices of A and B. This is one of our motivation points to conduct a systematic study of IWR(A, B)for 2×2 matrices, to be done in the next section, as they are smallest submatrices that can be used to show non-word-representability of $G^k(A, B)$ for some A, Band k.

2.3 Classification of word-representable split graphs defined by iteration of morphisms using two 2×2 matrices

A summary of our classification of word-representability of $G^k(A, B)$ for 2×2 matrices A and B can be found in Tables 2.1, 2.2, 2.3 and 2.4, where the index of word-representability IWR(A, B) is given along with a reference, or a comment to the respective result.

The cases when A is not an all-one matrix

For any 2×2 matrices A and B, the graph $G^1(A, B)$ is a split graph of order 4 which is always word-representable. Then, $IWR(A, B) \ge 2$. However, 2×2 matrices A and B such that $G^2(A, B)$ is non-word-representable can be found.

Proposition 39. For
$$A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$
 and $B = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$, IWR $(A, B) = 2$.
Proof. We have $M^2(A, B) = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$. Reordering columns of $M^2(A, B)$ in order given by the permutation 2314 yields the matrix $\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$. So, by The-

orem 23, $G^2(A, B)$ is non-word-representable ($G^2(A, B)$ contains T_1 as an induced subgraph).

Remark 40. Permuting rows or/and columns in A and B similarly to Proposition 39, we see that IWR(A, B) = 2 for A and B in Cases 31, 45, 81 and 101 in Tables 2.1, 2.2, 2.3 and 2.4 (in Case 81 G²(A, B) contains T₃, and in the other cases G²(A, B) contain T₁).

Proposition 41. For
$$A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$
 and $B = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$, $IWR(A, B) = 3$.

Proof. We have

$$M^{2}(A,B) = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } M^{3}(A,B) = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Reordering columns of $M^2(A, B)$ in order given by the permutation 4231 yields the

matrix $\begin{vmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{vmatrix}$. By Theorem 24, we have $G^2(A, B)$ is word-representable.

However, we have shown in Example 27 that $G^3(A, B)$ is non-word-representable. So IWR(A, B) = 3.

Remark 42. Proposition 41 gives Case 4 in Table 2.1. In each of Cases 5, 10, 11, 12, 14, 15, 17, 57, 66, 67, 68, 71, 72, 77, 78, 89, 99, 102, 104, 106, 108, 109, 111 and 112 in Tables 2.1, 2.2, 2.3 and 2.4, $M^2(A, B)$ has a permutation satisfying the conditions of Theorem 35 and $M^3(A, B)$ does not (similarly to Proposition 41). So IWR(A, B) = 3 for A and B in these cases. Moreover, by Theorem 35, column and row permutations of A and B give the same IWR. Consequently, we also have IWR(A, B) = 3 for A and B in Cases 19, 22, 24, 25, 28, 29, 32, 33, 36, 37, 39, 40, 42, 46, 47, 49, 58, 69, 70, 75, 76, 79, 80 and 90.

Proposition 43. For
$$A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$
 and $B = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$, $IWR(A, B) = 4$.

Proof. We have

$$M^{3}(A,B) = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Reordering columns of $M^3(A, B)$ in order given by the permutation 51732648

	0	1	1	1	0	0	0	0	
	0	0	0	0	0	1	0	0	
	1	1	1	0	0	0	0	0	
violds the matrix	0	0	0	0	0	0	1	0	
yields the matrix	0	0	1	1	0	0	0	0	
	0	0	0	0	1	1	0	0	
	1	1	1	1	0	0	0	0	
	0	0	0	0	0	0	0	0	

By Theorem 24, we have $G^3(A, B)$ is word-representable. For

suppose that a reordering of columns $\rho = \rho_1 \rho_2 \cdots \rho_{16}$ exists showing word-representability of $G^4(A, B)$ by Theorem 25. Then,

,

- from row 3, columns 1, 3, 5, 7, 9, 13 and 15 must be (cyclically) consecutive;
- from row 5, columns 3, 5, 7, 11 and 15 must be (cyclically) consecutive;
- from row 7, columns 1, 3, 5, 9, 11, 13 and 15 must be (cyclically) consecutive.

But then, from the first and the third bullet points, columns 1, 3, 5, 9, 13 and 15 must be consecutive and then column 7 or 11 is next to the left of them and the other one is next to the right of them. This contradicts to the second bullet

point. So there is no such ρ and $G^4(A, B)$ is non-word-representable. Therefore, IWR(A, B) = 4.

Remark 44. Proposition 43 gives Case 6 in Table 2.1. In each of Cases 53, 63, 83, 87, 93, 98 and 105 in Tables 2.1, 2.2, 2.3 and 2.4, $M^3(A, B)$ has a permutations satisfying condition in Theorem 35 but $M^4(A, B)$ does not (similarly to Proposition 43). So IWR(A, B) = 4 for A and B in these cases. Moreover, by Theorem 35, column and row permutations of A and B give the same IWR. Consequently, we also have IWR(A, B) = 3 for A and B in Cases 21, 35, 54, 64, 85, 92 and 95.

By Remarks 40, 42 and 44, we can see that in many cases the index of word-representability is 2, 3 or 4. Next, we will introduce certain definitions and theorems to present the cases where the index of word-representability is infinity.

Let M be an $m \times n$ binary matrix. For convenience, we will represent rows of M by binary strings of length n. For example, we will represent three rows of $\begin{bmatrix} 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ by 1101, 0100 and 0001.

Definition 45. Let A and B be $m \times n$ binary matrices. Define $R^k(A, B)$ to be the set of binary strings representing rows of $M^k(A, B)$. So every element of $R^k(A, B)$ is a binary string of length n^k . Each element of $R^k(A, B)$ is called a row pattern of $M^k(A, B)$.

Definition 46. Let $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ and $B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$ be 2 × 2 binary matrices and \mathcal{B}^n be the set of binary strings of length n. We define functions $u_{A,B} : \{0,1\} \rightarrow \mathcal{B}^2$ and $l_{A,B} : \{0,1\} \rightarrow \mathcal{B}^2$ by

$$u_{A,B}(0) = a_{11}a_{12}, \ l_{A,B}(0) = a_{21}a_{22}, \ u_{A,B}(1) = b_{11}b_{12} \ and \ l_{A,B}(1) = b_{21}b_{22}.$$

Moreover, if $v = v_1 v_2 \cdots v_k \in \mathcal{B}^k$, $k \ge 2$, we extend the definition of the functions $u_{A,B}$ and $l_{A,B}$ to the case of $\mathcal{B}^k \to \mathcal{B}^{2k}$ by

$$u_{A,B}(v) = u_{A,B}(v_1)u_{A,B}(v_2)\cdots u_{A,B}(v_k)$$

and

$$l_{A,B}(v) = l_{A,B}(v_1)l_{A,B}(v_2)\cdots l_{A,B}(v_k).$$

When A and B are clear from the context, we can omit the subscript and write u and l instead of $u_{A,B}$ and $l_{A,B}$, respectively.

Example 47. Let $A = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$. Then we have $M^{3}(A, B) = \begin{bmatrix} 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$

$$u_{A,B}(0) = 11$$
 and $l_{A,B}(0) = 00.$

So, $R^1(A, B) = \{11, 00\}$. Now,

$$u_{A,B}(11) = 1010$$
 and $l_{A,B}(11) = 1010$
 $u_{A,B}(00) = 1111$ and $l_{A,B}(00) = 0000$

so $R^2(A, B) = \{1010, 1111, 0000\}$. Repeating the procedure one more time yields

$$u_{A,B}(1010) = 10111011$$
 and $l_{A,B}(1010) = 10001000$
 $u_{A,B}(1111) = 10101010$ and $l_{A,B}(1111) = 10101010$
 $u_{A,B}(0000) = 11111111$ and $l_{A,B}(0000) = 00000000$

So, all elements in $R^k(A, B)$ are obtained by applying $u_{A,B}$ and $l_{A,B}$ to every element in $R^{k-1}(A, B)$. The next theorem generalizes this observation, and it can be proved easily by induction.

Theorem 48. Let A and B be 2×2 binary matrices. Then

$$R^{k}(A,B) = \{f_{k}(\cdots f_{2}(f_{1}(0))\cdots)|f_{i} \in \{u_{A,B}, l_{A,B}\}\} \text{ for any } k \geq 1.$$

Definition 49. Let $v = v_1 v_2 \cdots v_k \in B^k$. Then, $\Gamma(v) := \{m \in \{1, 2, \dots, k\} | v_m = 1\}$.

In order to study row patterns, we introduce a relation \leq on B^n . Let $x = x_1x_2\cdots x_k$ and $y = y_1y_2\cdots y_k$ be in B^k . We say that $x \leq y$ if and only if $x_i = 1$ implies $y_i = 1$ for every $i \in \{1, 2, \ldots, k\}$. In other words, $x \leq y$ if and only if $\Gamma(x) \subseteq \Gamma(y)$. It is easy to see that \leq is reflexive, antisymmetric and transitive, and thus \leq is a partial order.

Theorem 50. Let A and B be $m \times n$ binary matrices. For any k > 1, if $(R^k(A, B), \leq)$ is a total order, then $G^k(A, B)$ is word-representable.

Proof. Let $R^k(A, B) = \{x_1, x_2, \dots, x_l\}$ where $l \ge 1$ and x_1, x_2, \dots, x_l are binary strings of length n^k . Since $(R^k(A, B), \le)$ is a total order, w.l.o.g., we assume that $x_1 \le x_2 \le \dots \le x_l$. That is $\Gamma(x_1) \subseteq \Gamma(x_2) \subseteq \dots \subseteq \Gamma(x_l)$. Let

$$D_{1} := \Gamma(x_{1}),$$

$$D_{2} := \Gamma(x_{2}) \setminus \Gamma(x_{1}),$$

$$D_{3} := \Gamma(x_{3}) \setminus \Gamma(x_{2}),$$

$$\vdots$$

$$D_{l} := \Gamma(x_{l}) \setminus \Gamma(x_{l-1}) \quad \text{and}$$

$$D_{l+1} := \{1, 2, \dots, n^{k}\} \setminus \Gamma(x_{l}).$$

If $D_j = \{i_{j,1}, i_{j,2}, \dots, i_{j,|D_j|}\}$ for $i_{j,1} < i_{j,2} < \dots < i_{j,|D_j|}$, then $\rho = i_{1,1}i_{1,2}\cdots i_{1,|D_1|}i_{2,1}i_{2,2}\cdots i_{2,|D_2|}\cdots i_{l,1}i_{l,2}\cdots i_{l,|D_l|}$

is a n^k -permutation. Let M^* be the matrix obtained by reordering columns of $M^k(A, B)$ according to the order given by ρ . Then we want to prove that every row of $M^*(A, B)$ is of the form 1^s0^t for some $s, t \ge 0$. Let $y = y_1y_2\cdots y_{n^k}$ be a row pattern of $M^k(A, B)$ and $y^* = y_1^*y_2^*\cdots y_{n^k}^*$ be the row pattern after reordering y. Since $y \in R^k(A, B)$, then $y = x_q$ for some $q \in \{1, 2, \ldots, l\}$. So $y_i = 1$ for all $i \in \Gamma(x_q)$ and $y_i = 0$ for all $i \notin \Gamma(x_q)$. That is, $\Gamma(y)$ is

$$\{i_{1,1}, i_{1,2}, \dots, i_{1,|D_1|}, i_{2,1}, i_{2,2}, \dots, i_{2,|D_2|}, \dots, i_{q,1}, i_{q,2}, \dots, i_{l,|D_q|}\}$$

Hence $y^* = 1^{s}0^t$ where $s = |D_1| + |D_2| + \cdots + |D_q|$ and $t = n^k - |D_1| - |D_2| - \cdots - |D_q|$. Therefore every row of $M^*(A, B)$ is of the form 1^s0^t . By Theorem 24, we have that $G^k(A, B)$ is word-representable. **Theorem 51.** Let A and B be 2×2 binary matrices. If $x \leq y$ implies $\{u_{A,B}(x), l_{A,B}(x), u_{A,B}(y), l_{A,B}(y)\}$ is pairwise comparable under \leq for binary strings x and y of the same length, then $G^k(A, B)$ is word-representable for any $k \geq 0$.

Proof. We will firstly prove that $R^k(A, B)$ is comparable under \leq , and then apply Theorem 50 to complete the proof. Assume $x \leq y$ implies $\{u_{A,B}(x), l_{A,B}(x), u_{A,B}(y), l_{A,B}(y)\}$ is pairwise comparable under \leq for any binary strings x and yof the same length. We prove by induction on k that $R^k(A, B)$ is comparable under \leq . Because $0 \leq 0$, we have $\{u_{A,B}(0), l_{A,B}(0)\} = R^1(A, B)$ is comparable under \leq . Suppose that $R^l(A, B)$ is comparable under \leq for some $l \geq 1$. Let $v, w \in R^{l+1}(A, B)$. Then

$$v = u_{A,B}(x)$$
 or $v = l_{A,B}(x)$ for some $x \in R^{l}(A,B)$

and

$$w = u_{A,B}(y)$$
 or $w = l_{A,B}(y)$ for some $y \in R^{l}(A, B)$

By induction hypothesis, w.l.o.g., we can assume that $x \leq y$. So, $\{u_{A,B}(x), l_{A,B}(x), u_{A,B}(y), l_{A,B}(y)\}$ is comparable and v and w belong to this set. Thus we have that v and w are comparable. Hence $R^k(A, B)$ is comparable under \leq for any $k \geq 0$. Hence, by Theorem 50, $G^k(A, B)$ is word-representable for any $k \geq 0$.

Theorem 52. Let A and B be 2×2 binary matrices. If $\{u_{A,B}(100), l_{A,B}(100), u_{A,B}(101), l_{A,B}(101)\}$ is comparable under \leq , then $G^k(A, B)$ is word-representable for any $k \geq 0$.

Proof. For convenience, we write u and l instead of $u_{A,B}$ and $l_{A,B}$, respectively. Suppose that $\{u(100), l(100), u(101), l(101)\}$ is comparable under \leq . Let x = $x_1x_2\cdots x_m$ and $y = y_1y_2\cdots y_m$ be binary strings of length m such that $x \leq y$. Also, let

$$R := \{i | x_i = 0, y_i = 0\},$$

$$S := \{i | x_i = 1, y_i = 1\} \text{ and }$$

$$T := \{i | x_i = 0, y_i = 1\}.$$

Note that R, S, T partition the set $\{1, 2, ..., m\}$. Since u(100) and l(100) are comparable, we have two cases to consider.

If $u(100) \leq l(100)$, then $u(1) \leq l(1)$ and $u(0) \leq l(0)$. So we have $u(101) \leq l(101)$ and it is impossible that $l(101) \leq u(100)$ and $l(100) \leq u(101)$. So there are four possible cases here, which are

$$u(100) \le u(101) \le l(100) \le l(101),$$

$$u(100) \le u(101) \le l(101) \le l(100),$$

$$u(101) \le u(100) \le l(101) \le l(100) \text{ and}$$

$$u(101) \le u(100) \le l(100) \le l(101).$$

Similarly, in the case of $l(100) \leq u(100)$, we have $l(1) \leq u(1)$ and $l(0) \leq u(0)$. So $l(101) \leq u(101)$ and $u(100) \nleq l(100)$ and $u(101) \nleq l(100)$. So we have four more cases, which are

$$l(100) \le l(101) \le u(100) \le u(101),$$

$$l(100) \le l(101) \le u(101) \le u(100),$$

$$l(101) \le l(100) \le u(101) \le u(100) \text{ and}$$

$$l(101) \le l(100) \le u(100) \le u(101).$$

Next, we will consider comparability of the set $\{u(x), l(x), u(y), l(y)\}$ in each case.

- $u(100) \leq u(101) \leq l(100) \leq l(101)$. So we have $u(0) \leq u(1) \leq l(0) \leq l(1)$. Note that $u(x_i) \leq u(y_i)$ and $l(x_i) \leq l(y_i)$ for any $i \in T$. Then $u(x) \leq u(y)$ and $l(x) \leq l(y)$. Since $u(y_i) \leq l(x_i)$ where *i* belongs to R, S or T, so $u(y) \leq l(x)$. Hence, $u(x) \leq u(y) \leq l(x) \leq l(y)$.
- $u(100) \leq u(101) \leq l(101) \leq l(100)$. So we have $u(0) \leq u(1) \leq l(1) \leq l(0)$. Note that $u(x_i) \leq u(y_i)$ and $l(y_i) \leq l(x_i)$ for any $i \in T$. Then $u(x) \leq u(y)$ and $l(y) \leq l(x)$. Since $u(y_i) \leq l(y_i)$ where *i* belongs to R, S or T, so $u(y) \leq l(y)$. Hence, $u(x) \leq u(y) \leq l(y) \leq l(x)$.
- $u(101) \leq u(100) \leq l(101) \leq l(100)$. So we have $u(1) \leq u(0) \leq l(1) \leq l(0)$. Note that $u(y_i) \leq u(x_i)$ and $l(y_i) \leq l(x_i)$ for any $i \in T$. Then $u(y) \leq u(x)$ and $l(y) \leq l(x)$. Since $u(x_i) \leq l(y_i)$ where *i* belongs to R, S or T, so $u(x) \leq l(y)$. Hence, $u(y) \leq u(x) \leq l(y) \leq l(x)$.
- $u(101) \leq u(100) \leq l(100) \leq l(101)$. So we have $u(1) \leq u(0) \leq l(0) \leq l(1)$. Note that $u(y_i) \leq u(x_i)$ and $l(x_i) \leq l(y_i)$ for any $i \in T$. Then $u(y) \leq u(x)$ and $l(x) \leq l(y)$. Since $u(x_i) \leq l(x_i)$ where *i* belongs to R, S or T, so $u(x) \leq l(x)$. Hence, $u(y) \leq u(x) \leq l(x) \leq l(y)$.
- $l(100) \leq l(101) \leq u(100) \leq u(101)$. So we have $l(0) \leq l(1) \leq u(0) \leq u(1)$. Note that $l(x_i) \leq l(y_i)$ and $u(x_i) \leq u(y_i)$ for any $i \in T$. Then $l(x) \leq l(y)$ and $u(x) \leq u(y)$. Since $l(y_i) \leq u(x_i)$ where i belongs to R, S or T, so $l(y) \leq u(x)$. Hence, $l(x) \leq l(y) \leq u(x) \leq u(y)$.
- $l(100) \leq l(101) \leq u(101) \leq u(100)$. So we have $l(0) \leq l(1) \leq u(1) \leq u(0)$. Note that $l(x_i) \leq l(y_i)$ and $u(y_i) \leq u(x_i)$ for any $i \in T$. Then $l(x) \leq l(y)$ and $u(y) \leq u(x)$. Since $l(y_i) \leq u(y_i)$ where i belongs to R, S or T, so $l(y) \leq u(y)$. Hence, $l(x) \leq l(y) \leq u(y) \leq u(x)$.

- $l(101) \leq l(100) \leq u(101) \leq u(100)$. So we have $l(1) \leq l(0) \leq u(1) \leq u(0)$. Note that $l(y_i) \leq l(x_i)$ and $u(y_i) \leq u(x_i)$ for any $i \in T$. Then $l(y) \leq l(x)$ and $u(y) \leq u(x)$. Since $l(x_i) \leq u(y_i)$ where i belongs to R, S or T, so $l(x) \leq u(y)$. Hence, $l(y) \leq l(x) \leq u(y) \leq u(x)$.
- $l(101) \leq l(100) \leq u(100) \leq u(101)$. So we have $l(1) \leq l(0) \leq u(0) \leq u(1)$. Note that $l(y_i) \leq l(x_i)$ and $u(x_i) \leq u(y_i)$ for any $i \in T$. Then $l(y) \leq l(x)$ and $u(x) \leq u(y)$. Since $l(x_i) \leq u(x_i)$ where *i* belongs to R, S or T, so $l(x) \leq u(x)$. Hence, $l(y) \leq l(x) \leq u(x) \leq u(y)$.

We can see that $\{u(x), l(x), u(y), l(y)\}$ is comparable in every case. By Theorem 51, $G^k(A, B)$ is word-representable for any $k \ge 0$.

Remark 53. Theorem 52 can be applied to check word-representability of $G^k(A, B)$. We can see that $\{u_{A,B}(100), l_{A,B}(100), u_{A,B}(101), l_{A,B}(101)\}$ is comparable under \leq in Cases 2, 7, 8, 13, 51, 56, 61, 84, 94, 100, 103, 107 and 113 in Tables 2.1, 2.2, 2.3 and 2.4. Then IWR $(A, B) = \infty$ for A and B in these cases. By Theorem 35, column and row permutations of A and B in these cases preserve the index of word-representability. So we also have IWR $(A, B) = \infty$ for A and B in Cases 18, 23, 27, 30, 34, 43, 44, 48, 52, 59, 62, 86 and 96.

Proposition 54. Let $A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. Then $G^k(A, B)$ is word-representable for any $k \ge 0$.

Proof. The case of k = 0 is trivial. For $k \ge 1$, we let $S_0^k := \emptyset$,

$$S_j^k := \{s \in \{1, 2, \dots, 2^k\} | s \equiv 2^{j-1} \pmod{2^j} \} \text{ for } j \in \{1, 2, \dots, k\}$$

and

$$T^{k} := \{x_{1}x_{2}\cdots x_{2^{k}} | x_{i} = \begin{cases} 0 \text{ if } i \notin S_{j}^{k}, \\ 1 \text{ if } i \in S_{j}^{k} \end{cases} \text{ for some } j \in \{0, 1, \dots, 2^{k}\}\}.$$

We claim that $R^k(A, B) = T^k$ for any $k \ge 1$ and prove it by induction on k. It is obvious in the case of k = 1 because $R^1(A, B) = \{00, 10\}$ while $S_0^1 = \emptyset$ and $S_1^1 = \{1\}$. Suppose l is a positive integer such that $R^l(A, B) = T^l$. Let $y \in R^{l+1}(A, B)$, then $y = u_{A,B}(z)$ or $y = l_{A,B}(z)$ for some $z \in R^l(A, B)$. Since $R^l(A, B) = T^l$, we have

$$z = z_1 z_2 \cdots z_{2^l} \text{ where } z_i = \begin{cases} 0 \text{ if } i \notin S_j^l, \\\\ 1 \text{ if } i \in S_j^l. \end{cases}$$

If $y = u_{A,B}(z)$, then $y = 1010\cdots 10$. That is, $y_i = \begin{cases} 0 \text{ if } i \notin S_1^{l+1}, \\ 1 \text{ if } i \in S_1^{l+1} \end{cases}$, and so

 $y \in T^{l+1}$. If $y = l_{A,B}(z)$, the number of 1's in y and z is identical because 0 is mapped to 00 and 1 is mapped to 01. We can see that $y_{2i} = 1$ if and only if $z_i = 1$. Hence,

$$y_i = \begin{cases} 0 \text{ if } i \notin S_{r+1}^{l+1}, \\ 1 \text{ if } i \in S_{r+1}^{l+1}. \end{cases}$$

So $R^{l+1}(A, B) \subseteq T^{l+1}$. Conversely, let $v = v_1 v_2 \cdots v_{2^{l+1}}$ where

$$v_i = \begin{cases} 0 \text{ if } i \notin S_t^{l+1}, \\ 1 \text{ if } i \in S_t^{l+1} \end{cases}$$

for some $t \in \{0, 1, \dots, l+1\}$. If t = 0, note that $v = 000 \cdots 0 = l_{A,B}(000 \cdots 0)$ and $000 \cdots 0 \in R^l(A, B)$, and so $v \in R^{l+1}(A, B)$. If t = 1, we have $v = 1010 \cdots 10 =$

 $u_{A,B}(\bar{v})$ for any $\bar{v} \in R^l(A, B)$. That is $v \in R^{l+1}(A, B)$. Suppose $t \in \{2, 3, \dots, l+1\}$ and $w = w_1 w_2 \cdots w_{2^l}$ be an element of T^l such that

$$w_{i} = \begin{cases} 0 \text{ if } i \notin S_{t-1}^{l}, \\ 1 \text{ if } i \in S_{t-1}^{l}. \end{cases}$$

By induction hypothesis, $w \in R^{l}(A, B)$. Note that $v = l_{A,B}(w)$ and then $v \in R^{l+1}(A, B)$. So we have $T^{l+1} \subseteq R^{l+1}(A, B)$. Hence we have already proved the claim.

Note that $\{1, 2, \ldots, 2^k - 1\}$ is a disjoint union of S_1, S_2, \ldots, S_k . If $S_j^k = \{i_{j,1}, i_{j,2}, \ldots, i_{j,|S_j^k|}\}$ for $i_{j,1} < i_{l,2} < \cdots < i_{j,|S_j^k|}$, then we can let ρ be the permutation

$$i_{1,1}i_{1,2}\cdots i_{1,|S_1^k|}i_{2,1}i_{2,2}\cdots i_{2,|S_2^k|}\cdots i_{k,1}i_{k,2}\cdots i_{k,|S_k^k|}2^k.$$

Since $R^k(A, B) = T^k$, then all 1's in each row pattern in $R^k(A, B)$ is in columns $i_{j,1}, i_{j,2}, \ldots, i_{1,|S_j^k|}$ for some 1 < j < k. Therefore we can see that every row of the matrix obtained by reordering columns of $M^k(A, B)$ according to the order given by ρ is of the form $0^a 1^b 0^c$ for some non-negative integers a, b and c. By Theorem 24, $G^k(A, B)$ is word-representable for ant $k \ge 1$.

Remark 55. Proposition 54 gives $IWR(A, B) = \infty$ for A and B in Case 9 in Tables 2.1. By Theorem 35, column and row permutations of A and B give the same IWR. Consequently, we also have $IWR(A, B) = \infty$ for A and B in Cases 26 and 41.

Proposition 56. Let $A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and $B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Then $G^k(A, B)$ is word-representable for any $k \ge 0$.

Proof. The case of k = 0 is trivial. For any binary string x, we define \bar{x} to be the binary string obtained by changing digits of x from 0 to 1 and from 1 to 0. We claim that, for $k \ge 1$, $R^k(A, B) = \{x, \bar{x}\}$ for some $x \in B^{2^k}$ and prove it by induction on k. As $R^1(A, B) = \{10, 01\}$ and $01 = \overline{10}$, the case of k = 1 is done. Suppose that k > 1 is a positive integer such that $R^k(A, B) = \{x, \bar{x}\}$ for some $x \in B^{2^k}$. Then $R^{k+1}(A, B) = \{u_{A,B}(x), l_{A,B}(x), u_{A,B}(\bar{x}), l_{A,B}(\bar{x})\}$. Note that $u_{A,B}(0) = l_{A,B}(1)$ and $u_{A,B}(1) = l_{A,B}(0)$. Then $u_{A,B}(x) = l_{A,B}(\bar{x})$ and $l_{A,B}(x) = u_{A,B}(\bar{x})$. So we have $R^{k+1}(A, B) = \{u_{A,B}(x), l_{A,B}(x)\}$. Since $u_{A,B}(0) = \overline{l_{A,B}(1)} = \overline{l_{A,B}(1)}$, we have $u_{A,B}(x) = \overline{l_{A,B}(x)}$. That is, $R^{k+1}(A, B) = \{u_{A,B}(x), \overline{u_{A,B}(x)}\}$. Hence we have proved the claim by induction.

So, for any $k \ge 1$, $R^k(A, B) = \{x, \overline{x}\}$ for some binary string x. Suppose that there are s 1's in x. Let ρ be a permutation such that reordering $\begin{bmatrix} x \end{bmatrix}$ according to the order giving by ρ make all 1's in x be together in the first s columns. Then reordering $\begin{bmatrix} \overline{x} \end{bmatrix}$ according to the order giving by ρ makes all 1's in x be together in the last $2^k - s$ columns. Hence each row of the matrix obtained by reordering $M^k(A, B)$ according to the order giving by ρ is $1^{s}0^{2^k-s}$ or $0^{s}1^{2^k-s}$. By Theorem 24, $G^k(A, B)$ is word-representable for any $k \ge 0$.

The case when A is the all-one matrix

There are only 16 cases when $A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$. If $B = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, we have $M^0(A, B) = \begin{bmatrix} 0 \end{bmatrix}$ and $M^k(A, B)$ is all-one matrix for any $k \ge 1$ which is word-representable by Theorem 24. The rest of this chapter, except Theorem 57, deals with the cases when B has at least one 0.

Theorem 57. Let $A = \begin{bmatrix} 1 \end{bmatrix}_{m \times n}$ and B be an $m \times n$ binary matrix. Then, $M^k(A, B)$

is a submatrix of $M^{k+2}(A, B)$, and $G^k(A, B)$ is an induced subgraph of $G^{k+2}(A, B)$, for any $k \ge 0$.

Proof. Since the case of B being an all-one matrix is trivial, we assume that B is not an all-one matrix. Let $B = \begin{bmatrix} b_{ij} \end{bmatrix}_{m \times n}$ and $b_{rs} = 0$ for some $1 \le r \le m$ and $1 \le s \le n$. We will prove by induction on k that $M^k(A, B)$ is contained in $M^{k+2}(A, B)$ as a submatrix by rows $(r-1)m^k + 1, (r-1)m^k + 2, \ldots, rm^k$ and columns $(s-1)n^k + 1, (s-1)n^k + 2, \ldots, sn^k$ for any $k \ge 0$.

Note that $M^0(A, B) = \begin{bmatrix} 0 \end{bmatrix}, M^1(A, B) = \begin{bmatrix} 1 \end{bmatrix}_{m \times n}$ and

$$M^{2}(A,B) = \begin{bmatrix} B & B & \cdots & B \\ B & B & \cdots & B \\ \vdots & \vdots & \ddots & \vdots \\ B & B & \cdots & B \end{bmatrix}.$$

Let $M^2(A, B) = [m_{ij}]$, then $m_{rs} = 0$. So $M^0(A, B)$ is a submatrix of $M^2(A, B)$ by row $(r-1)m^0 + 1$ and column $(s-1)n^0 + 1$.

Let $l \geq 1$ be an integer such that $M^{l}(A, B)$ is a submatrix of $M^{l+2}(A, B)$ by rows $(r-1)m^{k} + 1, (r-1)m^{k} + 2, \ldots, rm^{k}$ and columns $(s-1)n^{k} + 1, (s-1)n^{k} + 2, \ldots, sn^{k}$. For the next iteration of morphism applied to $M^{l+2}(A, B)$, it is easy to see that $M^{l}(A, B)$ in the rows $(r-1)m^{k} + 1, (r-1)m^{k} + 2, \ldots, rm^{k}$ and the columns $(s-1)n^{k} + 1, (s-1)n^{k} + 2, \ldots, sn^{k} M^{l+2}(A, B)$ is mapped to $M^{l+1}(A, B)$ in the rows $(r-1)m^{k+1} + 1, (r-1)m^{k+1} + 2, \ldots, rm^{k+1}$ and columns $(s-1)n^{k+1} + 1, (s-1)n^{k+1} + 2, \ldots, sn^{k+1}$ of $M^{l+3}(A, B)$. Hence, $M^{k}(A, B)$ is a submatrix of $M^{k+2}(A, B)$ for any $k \geq 0$.

We know from Theorem 57 that $G^0(A, B) \preceq G^2(A, B) \preceq G^4(A, B) \preceq \cdots$ and

 $G^1(A, B) \preceq G^3(A, B) \preceq G^5(A, B) \preceq \cdots$ where $G \preceq H$ means G is an induced subgraph of H. So we are interested in investigating the smallest integer l such that $G^l(A, B)$ is non-word-representable in both cases of l being even and l being odd. The cases 114, 119, 120, 123, 124 and 129 in Table 2.4 are given by using Proposition 34. Theorem 52 can be applied to Cases 125, 126, 127 and 128, and the index of word-representability in these cases is infinity. The following propositions discuss the remaining cases.

 $\begin{aligned} \mathbf{Proposition 58.} \ For \ A &= \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \ and \ B &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \ \mathrm{IWR}(A, B) = 3. \ Moreover, \\ G^k(A, B) \ is \ not \ word-representable \ for \ k \geq 3. \end{aligned}$ $\begin{aligned} Proof. \ \mathrm{Note \ that} \ M^2(A, B) &= \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \ \mathrm{and} \ B &= \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \ \mathrm{and} \ B &= \begin{bmatrix} 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ \end{bmatrix} .$

Reordering columns of $M^2(A, B)$ in order given by 1324 yields the matrix $\begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$.

By Theorem 24, $G^2(A, B)$ is word-representable. Let M^* be a matrix obtained from reordering columns of $M^3(A, B)$ and every row of M^* is of the form $0^r 1^s 0^t$ or $0^r 1^s 0^t$. Then, the set of row patterns of M^* is

{00111111, 11001111, 11110011, 11111100}

or

$\{01111110, 10011111, 11100111, 11111001\}.$

If the set of row patterns of M^* is {00111111, 11001111, 11110011, 11111100}, then the occurrences of 11001111 and 11111100 do not satisfy the condition (ii) in Theorem 25. So, $G^3(A, B)$ is non-word-representable. Similarly, if the set of row patterns of M^* is {0111110, 10011111, 11100111, 11111001}, then the presence of 10011111 and 11111001 implies $G^3(A, B)$ is non-word-representable.

Now we consider the word-representability of $G^4(A, B)$. We have

$$R^{4}(A,B) = \{1011101010111010, 0111010101110101, 1110101011101010, \\1101010111010101, 1010101110101011, 0101011101010111, \\1010111010101110, 0101110101011101\}.$$

In order to apply Theorem 25, we assume the existence of an order $\rho = \rho_1 \rho_2 \cdots \rho_{16}$ with the following properties:

from 1011101010111010 ∈ R⁴(A, B), columns 2, 6, 8, 10, 14 and 16 must be cyclically consecutive;

- from 1110101011101010 $\in R^4(A, B)$, columns 4, 6, 8, 12, 14 and 16 must be cyclically consecutive;
- from 1010101110101011 $\in R^4(A, B)$, columns 2, 4, 6, 10, 12 and 14 must be cyclically consecutive.

It follows from the first and the second bullet points that 6, 8, 14, and 16 must be consecutive and then, w.l.o.g., 2 and 10 are next to the left of them and then 4 and 12 are next to the right them That means that 2 and 4 cannot be cyclically consecutive, which contradicts the third bullet point. So there is no such ρ and $G^4(A, B)$ is non-word-representable. As $G^3(A, B)$ is non-word-representable, and the class of word-representable graphs is hereditary, by Theorem 57, $G^{2k+1}(A, B)$ is nonword-representable for any $k \geq 1$. Similarly, $G^{2k}(A, B)$ is non-word-representable for any $k \geq 2$ because $G^4(A, B)$ is non-word-representable. Therefore, $G^k(A, B)$ is not word-representable for $k \geq 3$.

Remark 59. Proposition 58 gives Case 121 in Tables 2.4, and we obtain IWR(A, B) =3 in Case 122 by a column and row permutation of A and B.

Proposition 60. For
$$A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$
 and $B = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$, $\text{IWR}(A, B) = 5$. Moreover, $G^k(A, B)$ is not word-representable for $k \ge 5$.

Proof. It is easy to see that $G^0(A, B)$, $G^1(A, B)$ and $G^2(A, B)$ are word-representable. Since reordering columns of $M^3(A, B)$ in order given by the permutation 26153748 yields a matrix satisfying the condition in Theorem 24, $G^3(A, B)$ is word-representable. Further, reordering columns of $M^4(A, B)$ in order given by the permutation

also yields a matrix satisfying the condition in Theorem 24, so $G^4(A, B)$ is word-representable.

Next, we consider $G^5(A, B)$. We use u and l instead of $u_{A,B}$ and $l_{A,B}$, respectively. In order to apply Theorem 25, we assume the existence of an order $\rho = \rho_1 \rho_2 \cdots \rho_{32}$ proving word-representability of $G^5(A, B)$.

- l(l(l(u(u(0))))) = 10111011101110111011101110111011 ∈ R⁵(A, B) so columns
 2, 6, 10, 14, 18, 22, 26 and 30 must be cyclically consecutive in ρ.
- l(u(u(l(l(0))))) = 10101010111111110101010111111111 ∈ R⁵(A, B) so columns
 2, 4, 6, 8, 18, 20, 22 and 24 must be cyclically consecutive in ρ.
- u(u(l(l(u(0))))) = 111100001111111111000011111111 ∈ R⁵(A, B) so columns
 5, 6, 7, 8, 21, 22, 23 and 24 must be cyclically consecutive in ρ.

It follows from the first and the second bullet points that 2, 6, 18, and 22 must be consecutive and then, w.l.o.g., 10, 14, 26 and 30 are next to the left of these numbers and 4, 8, 20 and 24 are next to the right them. Hence ρ contains

 $\{10, 14, 26, 30\}, \{2, 6, 18, 22\}, \{4, 8, 20, 24\}$

where numbers in $\{\}$ are consecutive in ρ but are in some unknown to us order. From the third bullet point, ρ contains

$$\{10, 14, 26, 30\}, \{2, 18\}, \{6, 22\}, \{8, 24\}, \{4, 20\}$$

We obtain a contradiction with the fourth bullet point. So there is no such ρ and $G^5(A, B)$ is non-word-representable.

Next, we consider word-representability of $G^6(A, B)$. In order to apply Theorem 25, we assume that there exist a permutation $\tau = \tau_1 \tau_2 \cdots \tau_{64}$ proving wordrepresentability of $G^6(A, B)$.

Since all odd columns must be cyclically consecutive in τ , there is a unique $s \in \{1, 2, ..., 64\}$ such that τ_s is odd and τ_{s+1} is even, where for s = 64, s + 1 := 1. From the second bullet point, we have

$$\{\tau_s, \tau_{s-1}, \dots, \tau_{s-15}\} = \{1, 3, 5, \dots, 15, 33, 35, 37, \dots, 47\}$$

and
$$\{\tau_{s+1}, \tau_{s+2}, \dots, \tau_{s+16}\} = \{2, 4, 6, \dots, 16, 34, 36, 38, \dots, 48\}$$

where for $i \ge 0$, $\tau_{-i} := \tau_{64-i}$ and for $s+i \ge 65$, s+i := s+i-64. On the other hand, from the third bullet point, we have

$$\{\tau_s, \tau_{s-1}, \dots, \tau_{s-7}\} = \{3, 11, 19, 27, 35, 43, 51, 59\}$$

and
$$\{\tau_{s+1}, \tau_{s+2}, \dots, \tau_{s+8}\} = \{4, 12, 20, 28, 36, 44, 52, 60\}$$

where the indices less than 1 and larger than 64 are treated as above. We obtain a contradiction because $19 \notin \{\tau_s, \tau_{s-1}, \ldots, \tau_{s-15}\}$ but $19 \in \{\tau_s, \tau_{s-1}, \ldots, \tau_{s-7}\}$. Hence, there is no such τ and $G^6(A, B)$ is non-word-representable. Since the graphs $G^5(A, B)$ and $G^6(A, B)$ are not word-representable and the class of wordrepresentable graphs is hereditary, by Theorem 57, $G^k(A, B)$ is non-word-representable for any $k \geq 5$.

Remark 61. Proposition 60 is Case 117 in Table 2.4. By Theorem 35, column and row permutations of A and B give the same IWR. Consequently, we also have IWR(A, B) = 5 for A and B in Cases 115, 116 and 117.

2.4 Concluding remarks

This chapter is a major contribution to the study of word-representability of split graphs. Two key achievements in the chapter are as follows:

- Theorem 25 can be used to study word-representability of split graphs via adjacency matrices, which is a novel approach.
- Necessary conditions for word-representability of split graphs obtained by iteration of morphism can be checked in polynomial time. Indeed, for a given such graph defined by matrices A and B, we can go through all of 2×2 submatrices in A, and the respective submatrices in B, and then use our classification results in Tables 2.1, 2.2, 2.3 and 2.4 to detect non-word-representability.

As for open directions of research, it would be useful to provide a classification, similar to that we provided for 2×2 matrices in Tables 2.1, 2.2, 2.3 and 2.4, for larger matrices, for example, for 2×3 matrices, or 3×3 matrices, etc. This would enlarge our knowledge of word-representable split graphs obtained by iteration of morphisms, and hopefully, will eventually lead to a complete classification of such graphs.

For another research question, we noted in Tables 2.1, 2.2, 2.3 and 2.4 that if $G^5(A, B)$ is word-representable, then $IWR(A, B) = \infty$. In other words, the largest finite IWR in the case of 2×2 matrices is 5. Is there a reason for that? Does there exist a positive integer t (a constant, or a function of n and m) making the following statement true "If A, B are $n \times m$ matrices and $G^t(A, B)$ is wordrepresentable, then $IWR(A, B) = \infty$ "?

Finally, recall that if the leftmost bottom entry of A is 1 then $\lim_{k\to\infty} M^k(A, B)$ may not be well-defined as the sequence of graphs $G^k(A, B)$, for $k \ge 0$, may not be a chain of induced subgraphs. In all such cases, for 2×2 matrices, we still have that non-word-representability of $G^k(A, B)$ implies non-word-representability of $G^{k+1}(A, B)$. Is it always the case for $m \times n$ matrices A and B? If not, then how do we characterize the situations when it is the case?

Case	A	B	IWR(A, B)	Ref.	Case	A	B	IWR(A, B)	Ref.
1	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	* *	∞	A = 0					
2	$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	∞	Prop. 34	18	$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	∞	Prop. 34
3		$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	∞	Cor. 32	19		$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	3	Rem. 42
4		$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$	3	Pro. 41	20		$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$	∞	Cor. 32
5		$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	21		$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$	4	Rem. 44
6		$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	4	Prop. 43	22		$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42
7		$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$	∞	Rem 53	23		$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$	∞	Rem 53
8		$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$	∞	Rem 53	24		$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42
9		$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	∞	Prop 54	25		$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42
10		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	26		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	∞	Rem 55
11		$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42	27		$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$	∞	Rem 53
12		$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	28		$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42
13		$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$	∞	Rem 53	29		$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42
14		$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42	30		$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$	∞	Rem 53
15		$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	31		$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$	2	Rem. 40
16		$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$	2	Prop. 39	32		$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42
17		$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	33		$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42

Table 2.1: The index of word-representability of infinite split graphs G(A, B) for 2×2 matrices A and B.

Case	A	B	IWR (A, B)	Ref.	Case	A	B	IWR(A, B)	Ref.
34	$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	∞	Prop. 34	50	$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	∞	Prop. 34
35		$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	4	Rem. 44	51		$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	∞	Rem 53
36		$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$	3	Rem. 42	52		$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$	∞	Rem 53
37		$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	53		$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$	4	Rem. 44
38		$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	∞	Cor. 32	54		$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	4	Rem. 44
39		$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$	3	Rem. 42	55		$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$	∞	Cor. 32
40		$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	56		$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$	∞	Rem 53
41		$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	∞	Rem 55	57		$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42
42		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	58		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42
43		$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$	∞	Rem 53	59		$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$	∞	Rem 53
44		$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$	∞	Rem 53	60		$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$	∞	Prop. 34
45		$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$	2	Rem. 40	61		$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$	∞	Rem 53
46		$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42	62		$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$	∞	Rem 53
47		$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	63		$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$	4	Rem. 44
48		$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$	∞	Rem 53	64		$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$	4	Rem. 44
49		$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	65		$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$	∞	Prop. 34

Table 2.2: The index of word-representability of infinite split graphs G(A, B) for 2×2 matrices A and B.

Case	А	В	IWR (A, B)	Ref.	Case	А	В	IWR(A, B)	Ref.
66	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	3	Rem. 42	82	$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	∞	Prop. 34
67		$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	3	Rem. 42	83		$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	4	Rem. 44
68		$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$	3	Rem. 42	84		$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$	∞	Rem 53
69		$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	85		$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$	4	Rem. 44
70		$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42	86		$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$	∞	Rem 53
71		$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$	3	Rem. 42	87		$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$	4	Rem. 44
72		$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	88		$\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$	∞	Prop. 34
73		$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	∞	Cor. 32	89		$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42
74		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	∞	Prop 56	90		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42
75		$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42	91		$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$	∞	Cor. 32
76		$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	92		$\begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$	4	Rem. 44
77		$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$	3	Rem. 42	93		$\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$	4	Rem. 44
78		$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$	3	Rem. 42	94		$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$	∞	Rem 53
79		$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	95		$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$	4	Rem. 44
80		$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$	3	Rem. 42	96		$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$	∞	case 94
81		$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$	2	Rem. 40	97		$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$	∞	Prop. 34

Table 2.3: The remaining cases of the index of word-representability of infinite split graphs G(A, B) for 2×2 matrices A and B.

98	$\begin{bmatrix} 1\\ 0 \end{bmatrix}$	1 1	0 0	0 0	4	Rem. 44	114	$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	1 1	$\begin{bmatrix} 0\\ 0 \end{bmatrix}$	$\begin{bmatrix} 0\\ 0 \end{bmatrix}$	∞	Prop. 34
99			$\begin{bmatrix} 1\\ 0 \end{bmatrix}$	0 0	3	Rem. 42	115			$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$	$\begin{array}{c} 0\\ 0 \end{array}$	5	Rem. 61
100			0 0	$1 \\ 0$	∞	Rem 53	116			0 0	$\begin{array}{c} 1\\ 0 \end{array}$	5	Rem. 61
101			0 1	0 0	2	Rem. 40	117			$\begin{bmatrix} 0\\1 \end{bmatrix}$	$\begin{array}{c} 0\\ 0 \end{array}$	5	Prop. 60
102			0 0	$\begin{array}{c} 0 \\ 1 \end{array}$	3	Rem. 42	118			$\begin{bmatrix} 0\\ 0 \end{bmatrix}$	$\begin{bmatrix} 0\\1 \end{bmatrix}$	5	Rem. 61
103			$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$	1 0	8	Rem 53	119			$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1\\ 0 \end{bmatrix}$	∞	Prop. 34
104			$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	0 0	3	Rem. 42	120			$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	$\begin{bmatrix} 0\\ 0 \end{bmatrix}$	∞	Prop. 34
105			$\begin{bmatrix} 1\\ 0 \end{bmatrix}$	$\begin{array}{c} 0 \\ 1 \end{array}$	4	Rem. 44	121			$\begin{bmatrix} 1\\ 0 \end{bmatrix}$	$\begin{array}{c} 0 \\ 1 \end{array}$	3	Prop. 58
106			$\begin{bmatrix} 0\\1 \end{bmatrix}$	$1 \\ 0$	3	Rem. 42	122			$\begin{bmatrix} 0\\1 \end{bmatrix}$	$\begin{array}{c} 1\\ 0 \end{array}$	3	Rem. 59
107			0 0	1 1	∞	Rem 53	123			00	$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	∞	Prop. 34
108			$\begin{bmatrix} 0\\1 \end{bmatrix}$	$\begin{array}{c} 0 \\ 1 \end{array}$	3	Rem. 42	124			$\begin{bmatrix} 0\\1 \end{bmatrix}$	$\begin{bmatrix} 0\\1 \end{bmatrix}$	∞	Prop. 34
109			1 1	$\begin{array}{c} 1\\ 0\end{array}$	3	Rem. 42	125			$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	$\begin{pmatrix} 1 \\ 0 \end{bmatrix}$	∞	Thm. 52
110			$\begin{bmatrix} 1\\ 0 \end{bmatrix}$	1 1	8	Cor. 32	126			$\begin{bmatrix} 1\\ 0 \end{bmatrix}$	1 1	∞	Thm. 52
111			$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	$\begin{array}{c} 0 \\ 1 \end{array}$	3	Rem. 42	127			$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	$\begin{array}{c} 0 \\ 1 \end{array}$	∞	Thm. 52
112			$\begin{bmatrix} 0\\1 \end{bmatrix}$	1 1	3	Rem. 42	128			$\begin{bmatrix} 0\\1 \end{bmatrix}$	$\begin{array}{c} 1 \\ 1 \end{array}$	∞	Thm. 52
113			1 1	1 1	∞	Rem 53	129			$\begin{bmatrix} 1\\ 1 \end{bmatrix}$	1 1	∞	Prop. 34

Table 2.4: The remaining cases of the index of word-representability of infinite split graphs G(A, B) for 2×2 matrices A and B.

Chapter 3

Semi-transitivity of Directed Split Graphs Generated by Morphisms

In this chapter, based on [IK21], we study families of *directed* split graphs obtained by iterations of morphisms (involving three matrices A, B, C) applied to the adjacency matrices and giving as the limit infinite directed split graphs. For each of such a family we ask the question on whether all graphs in the family are oriented semi-transitively (i.e. are semi-transitive) or a finite iteration k of the morphism produces a non-semi-transitive orientation (which will stay non-semi-transitive for all iterations > k). In the former case, we say that the infinite split graph's index of semi-transitivity is ∞ (denoted IST $(A, B, C) = \infty$), and in the latter case it is k (assuming k is minimal possible).

The novelty of this research is in the study of directed graphs in connection to semi-transitive orientations, and in that we offer a way to generate interesting (from semi-transitivity point of view) families of directed split graphs using adjacency matrices and iterations of morphisms. This research will contribute to improving further known algorithms to recognise semi-transitive orientations



Figure 3.1: A guide to the classification results where A is assumed to have a 0 (a natural condition to ensure that our definitions work). For example, if none of A, B, C is a layered matrix then Theorem 82 is to be applied.

(on directed split graphs and beyond). It comes somewhat as a surprise that we were able to completely classify infinite directed split graphs with the index of semi-transitivity ∞ , where morphisms in question involve almost arbitrary $n \times m$ matrices over $\{-1, 0, 1\}$ as opposed to, say, 2×2 matrices in Chapter 2 (in a different context though); the only natural condition, to ensure that our definitions work, is that A has a 0. Our classification is done via several results depending on the structures of matrices A, B, C in question, and it is summarised in the diagram in Figure 3.1. Following the diagram, one can easily determine whether $IST(A, B, C) = \infty$ for any given A, B, C.

3.1 Adjacency matrix of directed split graphs

A directed graph is *semi-transitive* if its orientation is semi-transitive. The *adjacency matrix* $A = [a_{ij}]$ of a directed graph on n vertices is a binary matrix such that $a_{ij} = 1$ if $j \to i$ is an edge, and $a_{ij} = 0$ otherwise. Let $L(A) = [\ell_{ij}]$ be the $n \times n$ lower triangular matrix such that, for any i > j,

$$\ell_{ij} = \begin{cases} 1 & \text{if } a_{ij} = 1, \\ -1 & \text{if } a_{ji} = 1, \\ 0 & \text{otherwise} \end{cases}$$

and $\ell_{ij} = 0$ for any $i \leq j$.

Clearly, there is a one-to-one correspondence between directed graphs of order n and $n \times n$ lower triangular matrices over $\{-1, 0, 1\}$ with the diagonal elements equal 0. Thus, L(A) can play the role of the adjacency matrix of a directed graph. For i > j, the connectivity between vertices i and j is $j \to i$ if $\ell_{ij} = 1$, and is $i \to j$ if $\ell_{ij} = -1$, and there is no edge if $\ell_{ij} = 0$.

Example 62. If
$$A = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$
 is an adjacency matrix of a directed

 $\text{graph } G, \text{ then } L(A) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 1 & 0 \end{bmatrix} \text{ and the set of edges of } G \text{ (on 6)}$ $\text{vertices) is } \{1 \rightarrow 2, 2 \rightarrow 4, 1 \rightarrow 6, 5 \rightarrow 6, 3 \rightarrow 1, 5 \rightarrow 1, 4 \rightarrow 3, 6 \rightarrow 4\}.$

Our interest is in acyclically (without directed cycles) oriented split graphs since only such graphs have a chance to be semi-transitive. For any acyclically oriented split graph G, by Lemma 10, we know that the induced orientation of the maximal clique in G is transitive, so the following notion can be introduced.

Definition 63. An acyclically oriented split graph G with a maximal clique of order n is well-labelled if the vertex set of G is $V(G) = \{1, 2, ..., |V(G)|\}$ and the longest directed path in the maximal clique is $1 \rightarrow 2 \rightarrow \cdots \rightarrow n$.

Since we can relabel graphs, throughout the chapter, W.L.O.G. we can assume that any given acyclically oriented split graph is well-labelled. If A is the adjacency matrix for $S = (E_m, K_n)$ (where K_n is maximal) of order m + n, then

$$L(A) = \begin{bmatrix} L_n & O_{n,m} \\ M & O_m \end{bmatrix}$$

for some $m \times n$ matrix M, where $O_{n,m}$ and O_m are $n \times m$ and $m \times m$ zero matrices, respectively, and L_n is the $n \times n$ matrix such that all entries strictly below the main diagonal are 1's, and all other entries are 0's. Hence, every directed split graph with maximal clique of order n and independent set of order m can be represented by an $m \times n$ matrix M appearing in L(A) and recording directed edges between
K_n and E_m . Thus, generating a matrix M with entries in $\{-1, 0, 1\}$, we generate an acyclically oriented split graph.

Definition 64. Let $M = [m_{ij}]$ be an $m \times n$ matrix such that $m_{ij} \in \{-1, 0, 1\}$ for $1 \le i \le m$ and $1 \le j \le n$. Define

$$S_o(M) = \begin{bmatrix} L_n & O_{n,m} \\ M & O_m \end{bmatrix}$$

where the subscript o stands for "oriented" and S stands for "split". We denote the directed split graph corresponding to $S_o(M)$ by $G_o(M)$.

Example 65. If
$$M = \begin{bmatrix} 0 & 1 & 0 & 1 \\ -1 & 0 & -1 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$
 then
$$S_o(M) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

is the adjacency matrix of the directed graph $G_0(M)$ shown in Figure 3.2.

For convenience, we will represent rows of an $m \times n$ matrix M by strings of length n. For example, we will represent the three rows of $\begin{bmatrix} 1 & -1 & 0 & 1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ by 1(-1)01, 01(-1)0 and 0001.

Note that in Definition 64, the maximal clique of $G_o(M)$ is of order n + 1 if there is a row of the form $11 \cdots 1$ or $(-1)(-1) \cdots (-1)$ in M, and the maximal



Figure 3.2: The directed split graph $G_o(M)$ given by $S_o(M)$ in Example 65

clique is of order n otherwise. In the former case, $G_o(M)$ may not be well-labelled. In the case of n = 1, the graph $G_o(M)$ is a tree which is always semi-transitive. Thus, throughout this chapter, we can assume that $n \ge 2$.

Remark 66. If M is a zero matrix, then $G_o(M)$ is semi-transitive as it is a disjoint union of a transitively oriented clique and isolated vertices.

In what follows, x^r denotes $xx \cdots x$, where $x \in \{-1, 0, 1\}$ is repeated r times. For any $m \times n$ binary matrix M, we can consider the n columns of M as connectivity of the vertices in the maximal clique and m rows of M as connectivity of the vertices in the independent set. However, we note that M has the maximal clique of size n + 1 if there is a row of M having no 0. Then, we can move the vertex in the independent set which is connected to every vertices in the clique of size n to be one of the vertices in the maximal clique. However, we also have to concern about relabelling the vertices in the maximal clique to make sure that the split graph after moving the vertex is still well-labelled. In the case of $1^r(-1)^{n-r}$ is a row of M, we can create a new $(m-1) \times (n+1)$ binary matrix N such that the directed graphs G(M) and G(N) are the same and every row of N contains 0. This idea is used in the following lemma.

Lemma 67. Let $M := [m_{ij}]_{m \times n}$ be an $m \times n$ matrix over $\{-1, 0, 1\}$ such that $m_{p1} = m_{p2} = \cdots = m_{pr} = 1$ and $m_{p(r+1)} = m_{p(r+2)} = \cdots = m_{pn} = -1$ for some

$$p \in \{1, 2, \dots, m\}$$
 and $r \in \{0, 1, \dots, n\}$. If

	m_{11}	m_{12}	•••	m_{1r}	0	$m_{1(r+1)}$	•••	m_{1n}
N =	m_{21}	m_{22}		m_{2r}	0	$m_{2(r+1)}$	•••	m_{2n}
	:	÷		:	÷	:		÷
	$m_{(p-1)1}$	$m_{(p-1)2}$		$m_{(p-1)r}$	0	$m_{(p-1)(r+1)}$		$m_{(p-1)n}$
	$m_{(p+1)1}$	$m_{(p+1)2}$		$m_{(p+1)r}$	0	$m_{(p+1)(r+1)}$	•••	$m_{(p+1)n}$
	:	÷		:	:	÷		÷
	m_{m1}	m_{m2}		m_{mr}	0	$m_{m(r+1)}$		m_{mn}
is an $(m-1) \times (n+1)$ matrix, then $G_o(M)$ is isomorphic to $G_o(N)$.								

Proof. The p-th row in M, which is $1^r(-1)^{n-r}$, represents the vertex n + p in the independent set connected to all vertices in $K_n = \{1, 2, ..., n\}$. So K_n is not the maximal clique in $G_o(M)$, but $K_n \cup \{n + p\}$ is the maximal clique. Note that $\ell \to n + p$ for every vertex $\ell \in \{1, 2, ..., r\}$ and $n + p \to \ell$ for all vertex $\ell \in \{r + 1, r + 2, ..., n\}$. We relabel the vertex n + p to be r + 1 and relabel a vertex ℓ to be $\ell + 1$ for each $\ell \in \{r + 1, r + 2, ..., n + p - 1\}$. The relabelling gives the graph that can be represented by the matrix $S_o(N)$. Hence, $G_o(M)$ is isomorphic to $G_o(N)$.

Remark 68. Let M be an $m \times n$ matrix over $\{-1, 0, 1\}$. If $a_1a_2 \cdots a_n$ is the p-th row in M such that $a_q = -1$ and $a_r = 1$ for some $1 \leq q < r \leq n$, then $q \rightarrow r \rightarrow n + p \rightarrow q$ forms a cycle in $G_o(M)$. Hence, $G_o(M)$ is not semi-transitive if there is a 1 occurring to the right of a - 1 in a row in M. Consequently, if there is a row in M such that it has no 0 and it is not of the form $11 \cdots 1(-1)(-1) \cdots (-1)$, then $G_o(M)$ is not semi-transitive.

Let M be an $m \times n$ matrix over $\{-1, 0, 1\}$. We can see that the maximal clique of $G_o(M)$ is of order n or n + 1. Moreover, the maximal clique of $G_o(M)$ is the clique of order n + 1 if there is a row in M containing no 0. In this case, the matrix M does not represent only edges between vertices in the maximal clique and vertices in the independent set, but also a vertex in the maximal clique. By Remark 68, we can assume that M does not contain a row which has no 0 and is not of the form $1^r(-1)^{n-r}$ for some $0 \le r \le n$. Hence, if a row of M has no 0, it must be $1^r(-1)^{n-r}$ for some $1 \le r \le n$ for graph $G_o(M)$ to have a chance to be semi-transitive. Further, if $1^r(-1)^{n-r}$ is a row of M for some $0 \le r \le n$, by Lemma 67, we can consider the $(m-1) \times (n+1)$ matrix N in the statement of the lemma instead of M, and every row of N has a 0.

Theorem 69. Let M be an $m \times n$ matrix over $\{-1, 0, 1\}$. The directed split graph $G_o(M)$ is semi-transitive if and only if M satisfies the following conditions:

- (i) every row of M is of the form $0^r 1^s 0^t$ or $0^r (-1)^s 0^t$ or $1^r 0^s (-1)^t$ for $r, s, t \ge 0$;
- (ii) for each row of M of the form $1^a 0^b (-1)^c$ where a, b, c > 0, there is no other row having 1's in all positions from a to a + b + 1;
- (ii) for each row of M of the form $1^a 0^b (-1)^c$ where a, b, c > 0, there is no other row having (-1)'s in all positions from a to a + b + 1.

Proof. " \Leftarrow " Firstly, suppose that every row of M has a 0. Note that the vertices in the independent set will then be of types A, B and C, and taking into account conditions (ii) and (iii), Theorem 8 can be applied to see that $G_o(M)$ is semitransitive.

For the remaining case, suppose that there is a row p of M of the form $1^r (-1)^{n-r}$ where $1 \le p \le m$ and $0 \le r \le n$. Then, $\{1, 2, ..., n, n+p\}$ is the maximal clique in the directed graph $G_o(M)$. By Lemma 61, we have that $G_o(M)$ is isomorphic to $G_o(N)$, where N is the matrix obtained from M by deleting row p and adding a zero-column between columns r and r + 1 (in the cases of r = 0 and r = n, the zero-column will be the first column and the last column, respectively). Note that N still satisfies conditions (i) and (ii) and every row of N has a 0. Applying the first case, we have that $G_o(N)$ and $G_o(M)$ are semi-transitive.

" \Rightarrow " Firstly, suppose that every row of M has a 0. One can see that $G_o(M)$ is well-labelled, so the clique is oriented transitively and its longest path is $1 \rightarrow 2 \rightarrow$ $\cdots \rightarrow n$. Moreover, conditions (ii) and (iii) in Theorem 8 give conditions (i), (ii) and (iii) in this theorem.

For the remaining case, suppose that there is a row p of M of the form $1^{r}(-1)^{n-r}$ where $1 \leq p \leq m$ and $0 \leq r \leq n$. Then, $\{1, 2, \ldots, n, n+p\}$ is the maximal clique in the directed graph $G_o(M)$. By Lemma 61, we have that $G_o(M)$ is isomorphic to $G_o(N)$, where N is the matrix obtained from M by deleting row p and adding a zero-column between columns r and r + 1 (in the cases of r = 0 and r = n, the zero-column will be the first column and the last column, respectively). Since $G_o(M)$ is word-representable, then $G_o(n)$ is also word-representable. So N satisfies conditions (i), (ii) and (iii) in this theorem as every row of N has a 0. Therefore, every row of M, except for row p, satisfies (i), (ii) and (iii). For row p of M, if there is row q having 1's in r and r+1 position, then the row in N obtained from adding a 0 to row q of M does not satisfy the condition (i), which is a contradiction. Similarly, the occurrence of row q having (-1)'s in columns r and r+1 implies a contradiction. Hence M satisfies conditions (i), (ii) and (iii).

In this chapter, Theorem 69 plays an important role in determining if $G_o(M)$ is word-representable for a given matrix M. The following corollary is straightforward from Theorem 69. **Corollary 70.** Let M be an $m \times n$ matrix over $\{-1, 0, 1\}$. If every row of M is of the form $0^r 1^s 0^t$ or $0^r (-1)^s 0^t$ for $r, s, t \ge 0$, then the graph $G_o(M)$ is semi-transitive.

Definition 71. A matrix M is said to be a layered matrix if all entries in the same row of M are identical.

The next result is a straightforward corollary of Corollary 70.

Corollary 72. Let M be an $m \times n$ matrix over $\{-1, 0, 1\}$. If M is a layered matrix, then $G_o(M)$ is semi-transitive.

3.2 Directed split graphs generated by iterations of morphisms

Definition 73. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$. The matrix $M^k(A, B, C)$ is the k^{th} -iteration of the 2-dimensional morphism applied to the 1×1 matrix [0] which maps $[0] \rightarrow A$, $[1] \rightarrow B$ and $[-1] \rightarrow C$. Moreover, we write $S_o^k(A, B, C)$ for the matrix $S_o(M^k(A, B, C))$ and $G_o^k(A, B, C)$ for the graph with the adjacency matrix $S_o^k(A, B, C)$.

Example 74. Let
$$A = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix}$$
, $B = \begin{bmatrix} -1 & -1 \\ 1 & 0 \end{bmatrix}$ and $C = \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix}$. Then we have $M^0(A, B, C) = \begin{bmatrix} 0 \end{bmatrix}$, $M^1(A, B, C) = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix}$ and



Figure 3.3: The directed split graph $G_o^2(A, B, C)$ corresponding to the adjacency matrix $S_o^2(A, B, C)$ in Example 74.

$$M^{2}(A, B, C) = \begin{bmatrix} 0 & 1 & -1 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & -1 & -1 & -1 \end{bmatrix}. Hence, S_{o}^{2}(A, B, C) \text{ is the matrix}$$
$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & 0 & 0 & 0 \end{bmatrix}$$

and $G_o^2(A, B, C)$ is shown in Figure 3.3.

Remark 75. If A is a zero matrix, then $M^k(A, B, C)$ is always a zero matrix for any $m \times n$ matrices B and C and $k \ge 0$. Thus, by Remark 66, $G_o^k(A, B, C)$ is semi-transitive in this case. **Proposition 76.** If A, B and C are layered matrices over $\{-1, 0, 1\}$, then $G_o^k(A, B, C)$ is semi-transitive for any $k \ge 0$.

Proof. Let A, B and C be $m \times n$ matrices. Since every row in A, B and C is either 0^n or 1^n or $(-1)^n$, we have that every row in $M^k(A, B, C)$ is either 0^{n^k} or 1^{n^k} or $(-1)^{n^k}$, so by Corollary 72, $G_o^k(A, B, C)$ is semi-transitive.

If $A = [a_{ij}]_{m \times n}$ contains at least one 0, say $a_{ij} = 0$, then the entry in row i and column j of $M^1(A, B, C)$ is 0. By mapping this 0 to A in the next iteration of morphism, we obtain $A = M^1(A, B, C)$ as the $m \times n$ submatrix of $M^2(A, B, C)$ given by intersection of rows $(i-1)n+1, (i-1)n+2, \ldots, in$ and columns (j-1)m+2 $1, (j-1)m+2, \ldots, jm$. More generally, the $m^{k-1} \times n^{k-1}$ submatrix of $M^k(A, B, C)$ given by intersection of rows $(i-1)n^{k-1}+1, (i-1)n^{k-1}+2, \ldots, in^{k-1}$ and columns $(j-1)m^{k-1}+1, (j-1)m^{k-1}+2, \dots, jm^{k-1}$ is $M^{k-1}(A, B, C)$. So, we can consider the bottommost, then leftmost zero in A as the start of a chain of induced subgraphs generated by the morphism. Thus, the limit $\lim_{k\to\infty} M^k(A, B, C)$, called a fixed point of the morphism, is well-defined. So, we have that $G_o^i(A, B, C)$ is an induced subgraph of $G_o^k(A, B, C)$ for $i \leq k$, and the notion of the infinite split graph $G_o(A, B, C)$ is well-defined in the case when A has a 0. Note that this is not a necessary condition for $G_o(A, B, C)$ to be well-defined (for example, A, B, C) could be all one matrices). We are interested in the smallest integer ℓ (possibly non-existing) such that $G_o^{\ell}(A,B,C)$ is not semi-transitive for given A,B and C(then $G_o^i(A, B)$ is not semi-transitive for $i \ge \ell$).

Definition 77. Let A, B, C be $m \times n$ matrices such that A has a 0 as an entry. The index of semi-transitivity IST(A, B, C) of an infinite directed split graph $G_o(A, B, C)$ is the smallest integer ℓ such that $G_o^{\ell}(A, B, C)$ is not semi-transitive. If such an ℓ does not exist, that is, if $G_o^{\ell}(A, B, C)$ is semi-transitive for all ℓ , then $\ell := \infty$.

Note that since $G_o^0(A, B, C)$ is a graph with one vertex for any A, B, C, we have $IST(A, B, C) \ge 1$.

Remark 78. It follows from Proposition 76 that $IST(A, B, C) = \infty$ if A, B and C are layered matrices.

The following three lemmas give sufficient conditions for A, B and C to have $IST(A, B, C) = \infty.$

Lemma 79. Let A, B and C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and $IST(A, B, C) = \infty$. Then,

- If A is not a layered matrix, then there is no row in M^k(A, B, C) containing two 0's for any k ≥ 0.
- If B is not a layered matrix, then there is no row in M^k(A, B, C) containing two 1's for any k ≥ 0.
- If C is not a layered matrix, then there is no row in M^k(A, B, C) containing two (−1)'s for any k ≥ 0.

Proof. We will prove the first bullet point; the other bullet points can be proved analogously.

Let $A = [a_{ij}]$ be an $m \times n$ matrix and a_{ir}, a_{is} be two entries in row *i* of Asuch that $a_{ir} \neq a_{is}$ where $1 \leq r < s \leq n$. Denote $\mu^k(i, j) \in \{-1, 0, 1\}$ the entry of $M^k(A, B, C)$ in row *i* and column *j*. Suppose that row *a* of $M^k(A, B, C)$ contains at least two 0's for some *k*, say $\mu^k(a, b) = \mu^k(a, c) = 0$ where b < c. Consider the intersection of rows (a-1)m + 1, (a-1)m + 2, ..., am and columns (b-1)n + 1, (b-1)n + 2, ..., bn in $M^{k+1}(A, B, C)$, which is the matrix A because $\mu^k(a,b) = 0$. Similarly, the submatrix of $M^{k+1}(A, B, C)$ formed by rows (a-1)m + 1, (a-1)m + 2, ..., am and columns (c-1)n + 1, (c-1)n + 2, ..., cn is A. Hence, we have

$$\mu^{k+1}((a-1)m+i,(b-1)n+r) = \mu^{k+1}((a-1)m+i,(c-1)n+r) = a_{ir}$$

and

$$\mu^{k+1}((a-1)mi, (b-1)n+s) = \mu^{k+1}((a-1)m+i, (c-1)n+s) = a_{is}.$$

Thus, the submatrix of $M^{k+1}(A, B, C)$ formed by row (a-1)m + i and columns (b-1)n + r, (b-1)n + s, (c-1)n + r, (c-1)n + s is $[a_{ir}, a_{is}, a_{ir}, a_{is}]$. That is, row (a-1)m + i of $M^{k+1}(A, B, C)$ cannot be of the form $0^{r}1^{s}0^{t}$ or $0^{r}(-1)^{s}0^{t}$ or $1^{r}0^{s}(-1)^{t}$. By Theorem 69, $G_{o}^{k+1}(A, B, C)$ is not semi-transitive, which is a contradiction with $IST(A, B, C) = \infty$.

Lemma 80. Let A, B and C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and $IST(A, B, C) = \infty$. Then,

- If A and B are not layered matrices, then every entry of C is (-1).
- If A and C are not layered matrices, then every entry of B is 1.

Proof. Both statements are proved by similar arguments, so we will prove here only the first one. Suppose both A and B are not layered matrices. By Lemma 79, every row of $M^k(A, B, C)$ contains at most one 0 and at most one 1 for any $k \ge 2$. Then, there are at least $n^k - 2$ copies of (-1) in every row of $M^k(A, B, C)$. By Lemma 79, C is a layered matrix. Suppose that there is no (-1) in A and B. Since every row of $M^1(A, B, C) = A$ has at most one 0 and at most one 1 and no (-1), then n = 2 (recall our assumption of $n \ge 2$). Therefore, $M^2(A, B, C)$ has 4 columns with every row having more than one 0 or more than one 1, which is a contradiction.

If (-1) is an entry of A, then $M^1(A, B, C) = A$ has (-1) as an entry. So C is a submatrix of $M^2(A, B, C)$ as (-1) is mapped to C. Since every row of C has the same entries, and there is no more than one 0 and one 1 in each row of $M^2(A, B, C)$, we have that each entry of C must be (-1).

Finally, if there is no (-1) in A, but B contains (-1) as an entry, then $M^1(A, B, C) = A$ contains 1 as an entry. Since 1 maps to B, $M^2(A, B, C)$ contains B as a submatrix. So there is an entry (-1) in $M^2(A, B, C)$, and then C is a submatrix of $M^3(A, B, C)$. Since every row of C has entries equal to each other, and there is no more than one 0 and one 1 in each row of $M^2(A, B, C)$, then each entry of C is (-1).

Lemma 81. Let A, B and C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and $IST(A, B, C) = \infty$. If B and C are not layered matrices, then all entries of A are 0.

Proof. Suppose B and C are not layered matrices. By Lemma 79, every row of $M^k(A, B, C)$ contains at most one 1 and at most one (-1) for any $k \ge 2$. Then there are at least $n^k - 2$ zeroes in every row of $M^k(A, B, C)$. By Lemma 79, A is a layered matrix.

Assume that there is a row r in $A := [a_{ij}] = M^1(A, B, C)$ of the form $11 \cdots 1$. Also, suppose that a row s in $B := [b_{ij}]$ has two distinct entries, say $b_{sp} \neq b_{sq}$ for some $1 \le p < q \le n$. Note that the intersection of rows $(r-1)m + 1, (r-1)m + 2, \ldots, rm$ and columns $(\ell - 1)n + 1, (\ell - 1)n + 2, \ldots, \ell n$ in $M^2(A, B, C)$ is B for $\ell = 1, 2, \dots, m$. Then the submatrix of $M^2(A, B, C)$ formed by row (r-1)m + sand columns $p, q, n+p, n+q, 2n+p, 2n+q, \dots, (m-1)n+p, (m-1)n+q$ is

$$\begin{bmatrix} b_{sp} & b_{sq} & b_{sp} & b_{sq} & \cdots & b_{sp} & b_{sq} \end{bmatrix}.$$

Since every row of $M^k(A, B, C)$ has at most one 1 and at most one (-1) for any k, we have $b_{sp} = b_{sq} = 0$, which is a contradiction. Thus, there is no row in A of the form $11 \cdots 1$. Similarly, we can show that there is no row in A of the form $(-1)(-1) \cdots (-1)$. Hence, A is an all 0 matrix.

From Lemmas 80 and 81 we have the following theorem.

Theorem 82. Let A, B and C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0. If A, B and C are not layered, then IST(A, B, C) is finite.

Definition 83. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$. The triple (A, B, C) is said to be independent from B if there are no 1's in A and C. Similarly, the triple (A, B, C) is said to be independent from C if there are no (-1)'s in A and B.

For convenience, we write R(M) for the set of strings representing rows of M. Moreover, if A, B and C are $m \times n$ matrices over $\{-1, 0, 1\}$, then define $R^k(A, B, C)$ to be the set of strings representing rows of $M^k(A, B, C)$. So, every element of $R^k(A, B, C)$ is a string over $\{-1, 0, 1\}$ of length n^k . Each element of $R^k(A, B, C)$ is called a row pattern of $M^k(A, B, C)$.

Theorem 84. Let A, B and C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is independent from C. Then, $IST(A, B, C) = \infty$ if and only if A and B satisfy one of the following conditions, where $a_i \in \{0, 1\}$:

(1) A and B are layered matrices, or

$$(2) A = \begin{bmatrix} a_{1} & 1 & 1 & \cdots & 1 \\ a_{2} & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ a_{m} & 1 & 1 & \cdots & 1 \end{bmatrix} and B = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 & a_{1} \\ 1 & 1 & \cdots & 1 & a_{2} \\ \vdots & \vdots & & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & a_{m} \end{bmatrix} and B = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 & a_{m} \end{bmatrix}.$$

Proof. " \Leftarrow " There is no (-1) in A and B, and row patterns of $M^k(A, B, C)$ generated by A, B and C in (1), (2) and (3) are in the set

$$\{1^{n^k}, 0^{n^k}, 01^{n^{k-1}}, 1^{n^{k-1}}0\}$$

By Corollary 70, $M^k(A, B, C)$ is semi-transitive for all $k \ge 0$.

"⇒" Since (A, B, C) is independent from C, every entry of $M^k(A, B, C)$ is either 0 or 1. Assume IST $(A, B, C) = \infty$ and let $R(B) = \{b_1, b_2, \ldots, b_p\}$ where b_i is a binary string of length n. By Theorem 69, we have that every row of $M^k(A, B, C)$ is of the form $0^r 1^s 0^t$. If A is a layered matrix, then $R^1(A, B, C) \subseteq \{0^n, 1^n\}$ and

$$R^{2}(A, B, C) \subseteq \{0^{n^{2}}, 1^{n^{2}}, (b_{1})^{n}, (b_{2})^{n}, \dots, (b_{p})^{n}\}.$$

So, $R(B) \subseteq \{0^n, 1^n\}$ as otherwise, some strings in $R^2(A, B, C)$ are not of the form $0^r 1^s 0^t$. Thus, B is a layered matrix. Suppose A is not a layered matrix. By Lemma 79, $R^1(A, B, C) \subseteq \{01^{n-1}, 1^{n-1}0, 1^n\}$. If both 01^{n-1} and $1^{n-1}0$ are rows in A, then $1^{n-1}0(b_i)^{n-1}$ is a row pattern in $R^2(A, B, C)$ for some i. Since every row of $M^k(A, B, C)$ contains at most one 0, b_i must be 1^n , which contradicts $1^{n-1}0(b_i)^{n-1}$

not being of the form $0^r 1^s 0^t$. So, we have

$$A = \begin{bmatrix} a_1 & 1 & 1 & \cdots & 1 \\ a_2 & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & & \vdots \\ a_m & 1 & 1 & \cdots & 1 \end{bmatrix} \text{ or } A = \begin{bmatrix} 1 & 1 & \cdots & 1 & a_1 \\ 1 & 1 & \cdots & 1 & a_2 \\ \vdots & \vdots & & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & a_m \end{bmatrix}$$

where $a_i \in \{0, 1\}$. Note that each row of A is 1^n , 01^{n-1} or $1^{n-1}0$. If row i in A is 1^n , then row ((i-1)m+i) in $M^2(A, B, C)$ is x^n , where x is row i in B. Since x^n cannot contain more than one 0, we have $x = 1^n$. If row i in A is 01^{n-1} , then row ((i-1)m+i) in $M^2(A, B, C)$ is $01^{n-1}x^{n-1}$, where x is row i in B. So, $x = 1^n$ because $01^{n-1}x^{n-1}$ contains at most one 0. Similarly, if row i in A is $1^{n-1}0$, then row i in B is 1^n . Hence, B is an all 1 matrix.

Next theorem can be proved similarly to Theorem 84.

Theorem 85. Let A, B and C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is independent from B. Then, $IST(A, B, C) = \infty$ if and only if A and C satisfy one of the following conditions, where $a_i \in \{0, 1\}$:

(1) A and C are layered matrices, or

$$(2) A = \begin{bmatrix} a_1 & -1 & -1 & \cdots & -1 \\ a_2 & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots \\ a_m & -1 & -1 & \cdots & -1 \end{bmatrix} and C = \begin{bmatrix} -1 & -1 & \cdots & -1 \\ -1 & -1 & \cdots & -1 \\ \vdots & \vdots & & \vdots \\ -1 & -1 & \cdots & -1 \end{bmatrix}, or$$

$$(3) A = \begin{bmatrix} -1 & -1 & \cdots & -1 & a_1 \\ -1 & -1 & \cdots & -1 & a_2 \\ \vdots & \vdots & & \vdots & \vdots \\ -1 & -1 & \cdots & -1 & a_m \end{bmatrix} and C = \begin{bmatrix} -1 & -1 & \cdots & -1 \\ -1 & -1 & \cdots & -1 \\ \vdots & \vdots & & \vdots \\ -1 & -1 & \cdots & -1 \end{bmatrix}.$$

Theorem 86. Let A, B and C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is not independent from B and C. Suppose A is a layered matrix. Then, $IST(A, B, C) = \infty$ if and only if B and C are layered matrices.

Proof. Suppose IST $(A, B, C) = \infty$. The case when A is a zero matrix is trivial. Thus, assume that 1^n or $(-1)^n$ is a row in A. W.L.O.G., we suppose that 1^n is a row in $A = M^1(A, B, C)$. By Lemma 79, we have B is a layered matrix. If A also contains a row $(-1)^n$, then C is a layered matrix with the same reason. If A does not contain a row $(-1)^n$, then $(-1)^n$ must be a row of B because (A, B, C)is not independent from B and C. Since 1^n is a row of A, we have $BB \cdots B$ are m consecutive rows in $M^2(A, B, C)$. As $(-1)^n$ is a row in B, we have that $(-1)^{n^2}$ is a row in $M^2(A, B, C)$. By Lemma 79, C is a layered matrix.

For the converse direction, it is clear from Proposition 76 that if A, B and C are layered matrices, then $IST(A, B, C) = \infty$.

Definition 87. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$. The triple (A, B, C) is said to be

- an all-but-leftmost-negative triple if $R(A), R(B) \subseteq \{0(-1)^{n-1}, 1(-1)^{n-1}\}$ and C is an all (-1) matrix,
- an all-but-rightmost-negative triple if R(A), R(B) ⊆ {(-1)ⁿ⁻¹0, (-1)ⁿ⁻¹1}
 and C is an all (-1) matrix,
- an all-but-leftmost-positive triple if R(A), R(B) ⊆ {01ⁿ⁻¹, (-1)1ⁿ⁻¹} and C is an all 1 matrix,
- an all-but-rightmost-positive triple if R(A), R(B) ⊆ {1ⁿ⁻¹0, 1ⁿ⁻¹(-1)} and C is an all 1 matrix.

We can alternatively write Definition 87 as follow.

Definition 88. Let A, B, C are $m \times n$ matrices over $\{-1, 0, 1\}$. We define the triple (A, B, C) as following:

if

•
$$(A, B, C)$$
 is said to be all-but-leftmost-negative triple if

$$A = \begin{bmatrix} a_1 & -1 & -1 & \cdots & -1 \\ a_2 & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots \\ a_m & -1 & -1 & \cdots & -1 \end{bmatrix}$$
where $a_i \in \{0, 1\}$,

$$B = \begin{bmatrix} b_1 & -1 & -1 & \cdots & -1 \\ b_2 & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots \\ b_m & -1 & -1 & \cdots & -1 \end{bmatrix}$$
where $a_i \in \{0, 1\}$ and
C is an all (-1) matrix,

•
$$(A, B, C)$$
 is said to be all-but-leftmost-positive triple

$$A = \begin{bmatrix} a_1 & 1 & 1 & \cdots & 1 \\ a_2 & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ a_m & 1 & 1 & \cdots & 1 \end{bmatrix}$$
where $a_i \in \{0, -1\}$,

$$B = \begin{bmatrix} b_1 & 1 & 1 & \cdots & 1 \\ b_2 & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ b_m & 1 & 1 & \cdots & 1 \end{bmatrix}$$
where $a_i \in \{0, -1\}$ and
C is an all 1 matrix,

• (A, B, C) is said to be all-but-rightmost-negative triple if

$$A = \begin{bmatrix} -1 & -1 & \cdots & -1 & a_1 \\ -1 & -1 & \cdots & -1 & a_2 \\ \vdots & \vdots & & \vdots & \vdots \\ -1 & -1 & \cdots & -1 & a_m \end{bmatrix} \text{ where } a_i \in \{0, 1\},$$
$$B = \begin{bmatrix} -1 & -1 & \cdots & -1 & b_1 \\ -1 & -1 & \cdots & -1 & b_1 \\ -1 & -1 & \cdots & -1 & b_2 \\ \vdots & \vdots & & \vdots & \vdots \\ -1 & -1 & \cdots & -1 & b_m \end{bmatrix} \text{ where } a_i \in \{0, 1\} \text{ and }$$
$$C \text{ is an all } (-1) \text{ matrix,}$$

•
$$(A, B, C)$$
 is said to be all-but-rightmost-positive triple if

$$A = \begin{bmatrix} 1 & 1 & \cdots & 1 & a_1 \\ 1 & 1 & \cdots & 1 & a_2 \\ \vdots & \vdots & & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & a_m \end{bmatrix}$$
where $a_i \in \{0, -1\}$,

$$B = \begin{bmatrix} 1 & 1 & \cdots & 1 & b_1 \\ 1 & 1 & \cdots & 1 & b_1 \\ 1 & 1 & \cdots & 1 & b_2 \\ \vdots & \vdots & & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & b_m \end{bmatrix}$$
where $a_i \in \{0, -1\}$ and
C is an all 1 matrix.

From Definition 87 and 88, we can easily see that

• If (A, B, C) is all-but-leftmost-negative, then

$$R^{k}(A, B, C) \subseteq \{0(-1)^{n^{k}-1}, 1(-1)^{n^{k}-1}\},\$$

• If (A, B, C) is all-but-rightmost-negative, then

$$R^{k}(A, B, C) \subseteq \{(-1)^{n^{k}-1}0, (-1)^{n^{k}-1}1\},\$$

• If (A, B, C) is all-but-leftmost-positive, then

$$R^{k}(A, B, C) \subseteq \{01^{n^{k}-1}, (-1)1^{n^{k}-1}\},\$$

• If (A, B, C) is all-but-rightmost-positive, then

$$R^{k}(A, B, C) \subseteq \{1^{n^{k}-1}0, 1^{n^{k}-1}(-1)\}.$$

With this observation, we can prove the following theorem.

Theorem 89. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is not independent from B and C. Suppose A and B are not layered matrices and C is a layered matrix. Then, $IST(A, B, C) = \infty$ if and only if (A, B, C) is an all-but-leftmost-negative triple.

Proof. " \Leftarrow " Let (A, B, C) be all-but-leftmost-negative. Then, for any $k \ge 1$,

$$M^{k}(A, B, C) = \begin{bmatrix} x_{1} & -1 & -1 & \cdots & -1 \\ x_{2} & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & & \vdots \\ x_{m^{k}} & -1 & -1 & \cdots & -1 \end{bmatrix}$$

where $x_i \in \{0,1\}$. So $M^k(A, B, C)$ satisfies all conditions in Theorem 69, and hence $IST(A, B, C) = \infty$.

"⇒" Suppose IST(A, B, C) = ∞. From Lemma 80, we have that C is an all (-1) matrix. By Lemma 79, every row of $M^k(A, B, C)$ does not contain more than one 0 and more than one 1. Note that every row of A must be of the form $0^r 1^s 0^t$, $0^r (-1)^s 0^t$ or $1^r 0^s (-1)^t$, where $r, s, t \ge 0$. So, all possible row patterns of A are in

 $\{01, 10, 0(-1)^{n-1}, (-1)^{n-1}0, (-1)^n, 1(-1)^{n-1}, 10(-1)^{n-2}\}.$

Suppose that n = 2 and row *i* in *A* is 01. Then, the submatrix of $M^2(A, B, C)$ formed by rows $(i-1)m+1, (i-1)m+2, \ldots, im$ and columns 1, 2, 3, 4 is *AB*. So,

row (i-1)m+i in $M^2(A, B, C)$ is 01x, where x is row i in B. Note that 01x must be of the form $0^r 1^s 0^t$, where $r, s, t \ge 0$. Therefore, x is 11 because $M^2(A, B, C)$ contains at most one 0. So, 01x contains more than one 1, which contradicts Lemma 79. Hence, 01 cannot be a row in A. Similarly, we obtain that 10 is also not a row in A. Hence, we have that 01 and 10 cannot be a row in A.

Suppose row i in A is $10(-1)^{n-2}$. Then there is m consecutive rows in $M^2(A, B, C)$ built by $BACC \cdots C$. Note that row i in $BACC \cdots C$ is $y10(-1)^{n-2}zz \cdots z$, where y and z are rows i in B and C, respectively. Since $IST(A, B, C) = \infty$, $y10(-1)^{n-2}zz \cdots z$ must be of the form $1^r0^s(-1)^t$, where $r, s, t \ge 0$. Thus, $y = 1^n$ and $z = (-1)^n$. This contradicts to the fact that any row in $M^2(A, B, C)$ has at most one 1. Hence, $10(-1)^{n-2}$ cannot be a row in A.

Now, all possible row patterns of A are in

$$\{0(-1)^{n-1}, (-1)^{n-1}0, (-1)^n, 1(-1)^{n-1}\}.$$

If $1(-1)^{n-1}$ is not a row in A, then (A, B, C) is independent from C. Then $1(-1)^{n-1}$ must be a row in A. If $(-1)^{n-1}0$ or $(-1)^n$ is a row in A, then the condition (ii) of Theorem 69 is not satisfied. So, $G^1_o(A, B, C)$ is not semi-transitive.

Therefore $(-1)^{n-1}0$ and $(-1)^n$ are not rows in A and we have

$$A = \begin{bmatrix} a_1 & -1 & -1 & \cdots & -1 \\ a_2 & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & & \vdots \\ a_m & -1 & -1 & \cdots & -1 \end{bmatrix} \text{ where } a_i \in \{0, 1\}.$$

Since both $0(-1)^{n-1}$ and $1(-1)^{n-1}$ are rows in A, there are m consecutive rows of $M^2(A, B, C)$ built by $ACC \cdots C$ and $BCC \cdots C$. Then $1(-1)^{n^2-1}$ is a row in $M^2(A, B, C)$. Note that row i in $BCC \cdots C$ is $b_{i1}b_{i2} \cdots b_{in}(-1)^{n^2-n}$ where $b_{i1}b_{i2} \cdots b_{in}$ is row i in B. Since $M^2(A, B, C)$ is semi-transitive and $b_{i1}b_{i2} \cdots b_{in}(-1)^{n^2-n}$ is a row in $M^2(A, B, C)$, we have $b_{i1}b_{i2}\cdots b_{in}$ is $0^r(-1)^{n-r}$ or $10^s(-1)^{n-s-1}$ for some $0 \le r \le n$ and $0 \le s \le n-1$. As $M^2(A, B, C)$ contains at most one 0, we obtain that $b_{i1}b_{i2}\cdots b_{in}$ must be $1(-1)^{n-1}$ or $0(-1)^{n-1}$ or $10(-1)^{n-2}$ for any $1 \le i \le m$. If $10(-1)^{n-2}$ is a row of B, then there are m consecutive rows in $M^3(A, B, C)$ such that $ABCC\cdots C$ is its prefix. So, $x10(-1)^{n-2}yy\cdots y\cdots$ is a row in $M^3(A, B, C)$ where x is a row in A and y is a row in C. That is, $x = 1^n$, which is a contradiction. So, $10(-1)^{n-2}$ cannot be a row in B. Hence,

$$B = \begin{bmatrix} b_1 & -1 & -1 & \cdots & -1 \\ b_2 & -1 & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & & \vdots \\ b_m & -1 & -1 & \cdots & -1 \end{bmatrix} \text{ where } b_i \in \{0, 1\}.$$

Using similar arguments, we can prove the following theorem.

Theorem 90. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is not independent from B and C. Suppose A and C are not layered matrices and B is a layered matrix. Then, $IST(A, B, C) = \infty$ if and only if (A, B, C) is all-but-rightmost-positive.

By now, we already have classification for triples (A, B, C) with the index of semi-transitivity infinity except for the case when A is not a layered matrix and B and C are layered matrices and (A, B, C) is not independent from B, C. To solve the remaining cases, we need the following four lemmas.

Lemma 91. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is not independent from B and C. Then,

- (1) if 01^{n-1} and $1^{n-1}0$ are rows in A, then IST(A, B, C) is finite;
- (2) if $0(-1)^{n-1}$ and $(-1)^{n-1}0$ are rows in A, then IST(A, B, C) is finite;
- (3) if 01^{n-1} and $(-1)^{n-1}0$ are rows in A, then IST(A, B, C) is finite;
- (4) if $0(-1)^{n-1}$ and $1^{n-1}0$ are rows in A, then IST(A, B, C) is finite;
- (5) if $1^{p}0(-1)^{n-p-1}$ and $1^{q}0(-1)^{n-q-1}$ are rows in A, where $0 \le p < q \le n-1$, then IST(A, B, C) is finite.

Proof.

- (1) Suppose that IST(A, B, C) = ∞ and row i and row j in A are 01ⁿ⁻¹ and 1ⁿ⁻¹0, respectively. Note that Bⁿ⁻¹A gives m consecutive rows in M²(A, B, C) obtained by applying the morphism to 1ⁿ⁻¹0. Row i in Bⁿ⁻¹A is xⁿ⁻¹01ⁿ⁻¹, where x is row i in B. Since A is not a layered matrix, by Lemma 79, there is no 0 in x. So xⁿ⁻¹01ⁿ⁻¹ cannot be of the form 0^r1^s0^t, 0^r(-1)^s0^t or 1^r0^s(-1)^t. This contradicts to Theorem 69.
- (2) Suppose that $IST(A, B, C) = \infty$ and row *i* and row *j* in *A* are $0(-1)^{n-1}$ and $(-1)^{n-1}0$, respectively. Note that AC^{n-1} gives *m* consecutive rows in $M^2(A, B, C)$ obtained by applying the morphism to $0(-1)^{n-1}$. Row *j* in AC^{n-1} is $(-1)^{n-1}0x^{n-1}$, where *x* is row *j* in *B*. Since *A* is not a layered matrix, by Lemma 79, there is no 0 in *x*. So $(-1)^{n-1}0x^{n-1}$ cannot be of the form $0^r 1^s 0^t$, $0^r (-1)^s 0^t$ or $1^r 0^s (-1)^t$. This contradicts to Theorem 69.
- (3) Suppose that IST(A, B, C) = ∞ and row i and row j in A are 01ⁿ⁻¹ and (-1)ⁿ⁻¹0, respectively. Note that ABⁿ⁻¹ gives m consecutive rows in M²(A, B, C) obtained by applying the morphism to 01ⁿ⁻¹. Row j in ABⁿ⁻¹

is $(-1)^{n-1}0x^{n-1}$, where x is row j in B. Note that $(-1)^{n-1}0x^{n-1}$ must be of the form $0^r(-1)^s 0^t$, and so $x = 0^n$. Thus, $(-1)^{n-1}0x^{n-1} = (-1)^{n-1}0^{(n^2-n-1)}$ is a row in $M^2(A, B, C)$ having more than one 0, which contradicts to Lemma 79.

- (4) Suppose that IST(A, B, C) = ∞ and row i and row j in A are 0(-1)ⁿ⁻¹ and 1ⁿ⁻¹0, respectively. Note that ACⁿ⁻¹ gives m consecutive rows in M²(A, B, C) obtained by applying the morphism to 0(-1)ⁿ⁻¹. Row j in ACⁿ⁻¹ is 1ⁿ⁻¹0xⁿ⁻¹, where x is row j in C. Since A is not a layered matrix, by Lemma 79, there is no 0 in x. Therefore, 1ⁿ⁻¹0xⁿ⁻¹ is of the form 1^r0^s(-1)^t. So x = (-1)ⁿ and 1ⁿ⁻¹0xⁿ⁻¹ = 1ⁿ⁻¹0(-1)^{n²⁻ⁿ} is a row in M²(A, B, C). Note that Bⁿ⁻¹A gives m consecutive rows in M²(A, B, C) obtained by application of the morphism to 1ⁿ⁻¹0. Row j in Bⁿ⁻¹A is yⁿ⁻¹1ⁿ⁻¹0, where y is row j in B. Since A is not a layered matrix, by Lemma 79, there is no 0 in x. Therefore, 0ⁿ⁻¹A is yⁿ⁻¹1ⁿ⁻¹0, where y is row j in B. Since A is not a layered matrix, by Lemma 79, there is no 0 in y. Therefore, yⁿ⁻¹1ⁿ⁻¹0 is of the form 0^r1^s0^t. So y = 1ⁿ and yⁿ⁻¹1ⁿ⁻¹0 = 1^{n²-1}0 is a row in M²(A, B, C). Note that 1ⁿ⁻¹0(-1)^{n²-n-1} and 1^{n²-1}0 break the second condition of Theorem 69. Hence, G²_o(A, B, C) is not semi-transitive and this leads to a contradiction.
- (5) Suppose that $IST(A, B, C) = \infty$ and row *i* and row *j* in *A* are $1^{p}0(-1)^{n-p-1}$ and $1^{q}0(-1)^{n-q-1}$, respectively, where $0 \leq p < q \leq n-1$. Note that $B^{p}AC^{n-p-1}$ gives *m* consecutive rows in $M^{2}(A, B, C)$ obtained by applying the morphism to $1^{p}0(-1)^{n-p-1}$. Row *i* in $B^{p}AC^{n-p-1}$ is $x^{p}1^{p}0(-1)^{n-p-1}y^{n-p-1}$ where *x* is row *i* in *B* and *y* is row *i* in *C*. Since *A* is not a layered matrix, by Lemma 79, there is no more than one 0 in any row of $M^{2}(A, B, C)$. By Theorem 69, we obtain $x^{p}1^{p}0(-1)^{n-p-1}y^{n-p-1}$ equals $1^{np+p}0(-1)^{n^{2}-np-p-1}$. Note that $B^{q}AC^{n-q-1}$ gives *m* consecutive rows in $M^{2}(A, B, C)$ obtained by ap-

plication of the morphism to $1^{q}0(-1)^{n-q-1}$, and $x^{q}1^{q}0(-1)^{n-q-1}y^{n-q-1}$ is its row *i*. Similarly to the above, we have $x^{q}1^{q}0(-1)^{n-q-1}y^{n-q-1} = 1^{nq+q}0(-1)^{n^2-nq-q-1}$. That is, both $1^{np+p}0(-1)^{n^2-np-p-1}$ and $1^{nq+q}0(-1)^{n^2-nq-q-1}$ are rows of $M^2(A, B, C)$. If p = 0 and q = n-1, then $0(-1)^{n-1}$ and $1^{n-1}0$ are rows in A which is a contradiction by (4). So, one of $1^{np+p}0(-1)^{n^2-np-p-1}$ and $1^{nq+q}0(-1)^{n^2-nq-q-1}$ is of the form $1^r0^s(-1)^t$ for some r, s, t > 0. Note that $G_o^2(A, B, C)$ is not semitransitive because of the second condition of Theorem 69 is not satisfied, and this is a contradiction.

Lemma 92. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is not independent from B and C. Then,

- (1) if $1^{p}0(-1)^{n-p-1}$ and 01^{n-1} are rows in A, where $1 \leq p \leq n-2$, then IST(A, B, C) is finite;
- (2) if $1^{p}0(-1)^{n-p-1}$ and $0(-1)^{n-1}$ are rows in A, where $1 \le p \le n-2$, then IST(A, B, C) is finite;
- (3) if $1^{p}0(-1)^{n-p-1}$ and $1^{n-1}0$ are rows in A, where $1 \le p \le n-2$, then IST(A, B, C) is finite;
- (4) if $1^{p}0(-1)^{n-p-1}$ and $(-1)^{n-1}0$ are rows in A, where $1 \le p \le n-2$, then IST(A, B, C) is finite.

Proof.

(1) Suppose that $1^{p}0(-1)^{n-p-1}$ and 01^{n-1} are rows *i* and *j* in *A*, respectively, and $IST(A, B, C) = \infty$. Note that $B^{p}AC^{n-p-1}$ gives *m* consecutive rows in $M^{2}(A, B, C)$ obtained by applying the morphism to $1^{p}0(-1)^{n-p-1}$ in $M^1(A, B, C)$. Row j in B^pAC^{n-p-1} is $b^p01^{n-1}c^{n-p-1}$, where b and c are row j in B and C, respectively. So $b^p01^{n-1}c^{n-p-1}$ must be $0^r1^s0^t$ for some $r, s, t \ge 0$. Hence, $b = 0^n$ and $c = 1^n$. As A is not a layered matrix, every row in $M^2(A, B, C)$ contains at most one 0, which is a contradiction. Therefore, $IST(A, B, C) < \infty$.

- (2) This is given by (5) in Lemma 91.
- (3) This is given by (5) in Lemma 91.
- (4) Suppose that 1^p0(-1)^{n-p-1} and (-1)ⁿ⁻¹0 are rows *i* and *j* in *A*, respectively, and IST(*A*, *B*, *C*) = ∞. Note that B^pAC^{n-p-1} gives *m* consecutive rows in M²(*A*, *B*, *C*) obtained by applying the morphism to 1^p0(-1)^{n-p-1} in M¹(*A*, *B*, *C*). Row *j* in B^pAC^{n-p-1} is b^p(-1)ⁿ⁻¹0c^{n-p-1}, where *b* and *c* are row *j* in *B* and *C*, respectively. So, b^p(-1)ⁿ⁻¹0c^{n-p-1} must be 0^r(-1)^s0^t for some *r*, *s*, *t* ≥ 0. Hence, *b* = (-1)ⁿ and *c* = 0ⁿ. As *A* is not a layered matrix, every row in M²(*A*, *B*, *C*) contains at most one 0, which is a contradiction. Therefore, IST(*A*, *B*, *C*) < ∞.</p>

Definition 93. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$. A triple (A, B, C) is left-0-invariant if A, B, C satisfy the following properties:

- every row in A is in $\{01^{n-1}, 1^n, 0(-1)^{n-1}, (-1)^n\};$
- every row in B and C is in $\{1^n, (-1)^n\}$;
- if 01^{n-1} appears as a row in A, then
 - row i in A is 01^{n-1} implies row i in B is 1^n ;

- row i in A is 1^n implies row i in B is 1^n ;
- row i in A is $0(-1)^{n-1}$ implies row i in B is $(-1)^n$;
- row i in A is $(-1)^n$ implies row i in B is $(-1)^n$;
- if $0(-1)^{n-1}$ appears as a row in A, then
 - row i in A is 01^{n-1} implies row i in C is 1^n ;
 - row i in A is 1^n implies row i in C is 1^n ;
 - row i in A is $0(-1)^{n-1}$ implies row i in C is $(-1)^n$;
 - row i in A is $(-1)^n$ implies row i in C is $(-1)^n$.

Definition 94. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$. A triple (A, B, C) is right-0-invariant if A, B, C satisfy the following properties:

- every row in A is in $\{1^{n-1}0, 1^n, (-1)^{n-1}0, (-1)^n\};$
- every row of B and C is in $\{1^n, (-1)^n\}$;
- if $1^{n-1}0$ appears as a row in A, then
 - row i in A is $1^{n-1}0$ implies row i in B is 1^n ;
 - row i in A is 1^n implies row i in B is 1^n ;
 - row i in A is $(-1)^{n-1}0$ implies row iin B is $(-1)^n$;
 - row i in A is $(-1)^n$ implies row i in B is $(-1)^n$;
- if $(-1)^{n-1}0$ appears as a row in A, then
 - row i in A is $1^{n-1}0$ implies row i in C is 1^n ;
 - row i in A is 1^n implies row i in C is 1^n ;

- row i in A is
$$(-1)^{n-1}0$$
 implies row i in C is $(-1)^n$;

$$- row i in A is (-1)^n implies row i in C is (-1)^n.$$

Lemma 95. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0. Then,

- (1) If (A, B, C) is left-0-invariant and $01^{n-1} \notin R(A)$, then $01^{n^k-1} \notin R^k(A, B, C)$ for any $k \ge 0$.
- (2) If (A, B, C) is left-0-invariant and $0(-1)^{n-1} \notin R(A)$, then $0(-1)^{n^{k}-1} \notin R^{k}(A, B, C)$ for any k > 0.
- (3) If (A, B, C) is right-0-invariant and $1^{n-1}0 \notin R(A)$, then $1^{n^k-1}0 \notin R^k(A, B, C)$ for any k > 0.
- (4) If (A, B, C) is right-0-invariant and $(-1)^{n-1}0 \notin R(A)$, then $(-1)^{n^k-1}0 \notin R^k(A, B, C)$ for any k > 0.

Proof. As all of the statements are proved in similar ways, we will only prove (1). Assume (A, B, C) is left-0-invariant and $01^{n-1} \notin R(A)$. For k = 1, it is obvious that $M^1(A, B, C) = A$ and then $01^{n-1} \notin R^1(A, B, C)$. Suppose $k \ge 2$ and $01^{n^{k}-1} \in R^k(A, B, C)$. Let $0x_1x_2 \cdots x_{n^{k-1}-1}$ be a row in $M^{k-1}(A, B, C)$ such that applying to it the morphism creates row $01^{n^{k}-1}$. That is, $01^{n^{k}-1}$ is a row in the matrix $AX_1X_2 \cdots X_{n^{k-1}-1}$, where $X_i \in \{A, B, C\}$, obtained from $0x_1x_2 \cdots x_{n^{k-1}-1}$ by application of the morphism. This is a contradiction because $01^{n-1} \notin R(A)$. Hence, $01^{n^{k}-1} \notin R^k(A, B, C)$.

Lemma 96. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0. If (A, B, C) is left-0-invariant (resp., right-0-invariant), then $IST(A, B, C) = \infty$. Proof. Suppose that (A, B, C) is left-0-invariant. We will prove that for any k > 0, $R^k(A, B, C) \subseteq \{01^{n^k-1}, 1^{n^k}, 0(-1)^{n^{k-1}}, (-1)^{n^k}\}$ by induction on k. From the definition of a left-0-invariant tripple, we have that $R^1(A, B, C) = R(A) \subseteq \{01^{n-1}, 1^n, 0(-1)^{n-1}, (-1)^n\}$. Suppose $R^k(A, B, C) \subseteq \{01^{n^{k-1}}, 1^{n^k}, 0(-1)^{n^{k-1}}, (-1)^{n^k}\}$ for some k. If $01^{n-1} \notin R(A)$, then $0(-1)^{n-1} \in R(A)$ and, by Lemma 95, $01^{n^{k-1}} \notin R^k(A, B, C)$. So, every row in $M^k(A, B, C)$ is $1^{n^k}, 0(-1)^{n^{k-1}}$ or $(-1)^{n^k}$. As every row in $M^{k+1}(A, B, C)$ is a row in an $m \times n^{k+1}$ matrix obtained by applying the morphism to a row in $M^k(A, B, C)$, we have that

$$R^{k+1}(A, B, C) = R(B^{n^k}) \cup R(AC^{n^{k-1}}) \cup R(C^{n^k}).$$

We can see that $R(B^{n^k})$ and $R(C^{n^k})$ are subset of $\{1^{n^{k+1}}, (-1)^{n^{k+1}}\}$. Row *i* in $AC^{n^{k}-1}$ is $1^{n^{k+1}}, (-1)^{n^{k+1}}$ and $0(-1)^{n^{k+1}-1}$ if row *i* in *A* is $1^n, (-1)^n$ and $0(-1)^n$, respectively. Hence, $R^{k+1}(A, B, C) \subseteq \{1^{n^{k+1}}, 0(-1)^{n^{k+1}-1}, (-1)^{n^{k+1}}\}$ in the case of $01^{n-1} \notin R(A)$. For the case of $0(-1)^{n-1} \notin R(A)$, we can follow similar arguments to see that $R^{k+1}(A, B, C) \subseteq \{01^{n^{k+1}-1}, 1^{n^{k+1}}, (-1)^{n^{k+1}}\}$. Assume both 01^{n-1} and $0(-1)^{n-1}$ are in R(A). So, every row in $M^k(A, B, C)$ is $01^{n^{k}-1}, 1^{n^k}, 0(-1)^{n^{k-1}}$ or $(-1)^{n^k}$ and

$$R^{k+1}(A, B, C) = R(AB^{n^{k}-1}) \cup R(B^{n^{k}}) \cup R(AC^{n^{k}-1}) \cup R(C^{n^{k}}).$$

Note that $R(B^{n^k}), R(C^{n^k}) \subseteq \{1^{n^{k+1}}, (-1)^{n^{k+1}}\}$. Row i in AC^{n^k-1} is $1^{n^{k+1}}, (-1)^{n^{k+1}}, (01^{n^{k+1}-1} \text{ and } 0(-1)^{n^{k+1}-1}$ if row i in A is $1^n, (-1)^n, 01^n$ and $0(-1)^n$, respectively. Row i in AB^{n^k-1} is $1^{n^{k+1}}, (-1)^{n^{k+1}}, 01^{n^{k+1}-1}$ and $0(-1)^{n^{k+1}-1}$ if row i in A is $1^n, (-1)^n, 01^n$ and $0(-1)^n$, respectively. Hence, $R^{k+1}(A, B, C) \subseteq \{1^{n^{k+1}}, 0(-1)^{n^{k+1}-1}, (-1)^{n^{k+1}}\}$. Thus, we have shown that, for any k > 0,

$$R^{k}(A, B, C) \subseteq \{01^{n^{k}-1}, 1^{n^{k}}, 0(-1)^{n^{k}-1}, (-1)^{n^{k}}\}.$$

By Corollary 70, $G_o^k(A, B, C)$ is semi-transitive for any k > 0, which means that $IST(A, B, C) = \infty$.

Theorem 97. Let A, B, C be $m \times n$ matrices over $\{-1, 0, 1\}$ such that A has a 0 and (A, B, C) is not independent from B and C. Suppose A is not a layered matrix but B and C are layered matrices. Then, $IST(A, B, C) = \infty$ if and only if one of the following conditions holds:

- (A, B, C) is left-0-invariant.
- (A, B, C) is right-0-invariant.
- R(A) = {1^p0(−1)^{n−p−1}} for some p ∈ {1, 2, ..., n−2}, and B and C are all 1 and (−1) matrices, respectively.

Proof. Assume IST $(A, B, C) = \infty$. Since A is not a layered matrix, by Lemma 79, every row of $M^1(A, B, C) = A$ contains at most one 0. Then, every row in A is $01^{n-1}, 1^{n-1}0, 1^n, 0(-1)^{n-1}, (-1)^{n-1}0, (-1)^n, 1^p0(-1)^{n-p-1}$ or $1^q(-1)^{n-q}$ for some $p \in \{1, 2, ..., n-2\}$ and $q \in \{1, 2, ..., n-1\}$. Since (A, B, C) is not independent from B and C, and B and C are layered matrices, we have every row of B and C must be 1^n or $(-1)^n$, otherwise there is a row in $M^k(A, B, C)$ having more than one 0 for some k.

If $1^q(-1)^{n-q}$ is row *i* in *A* for $q \in \{1, 2, ..., n-1\}$, then every row in *A*, except for row *i*, is $1^q(-1)^{n-q}$, $1^{q-1}0(-1)^{n-q}$ or $1^q0(-1)^{n-q-1}$. By (5) in Lemma 91, we have that *A* cannot contain both $1^{q-1}0(-1)^{n-q}$ and $1^q0(-1)^{n-q-1}$ as its rows. If $1^{q-1}0(-1)^{n-q} \notin R(A)$, then

$$A = \begin{bmatrix} 1^{q} & a_{1} & (-1)^{n-q-1} \\ 1^{q} & a_{2} & (-1)^{n-q-1} \\ \vdots & \vdots & \vdots \\ 1^{q} & a_{m} & (-1)^{n-q-1} \end{bmatrix}$$

for $a_i \in \{0,1\}$. Since A has a 0, there is row j in A of the form $1^{q}0(-1)^{n-q-1}$. Let b and c be row j in B and C, respectively. Note that $B^q A C^{n-q-1}$ is m consecutive rows of M^2 obtained by applying the morphism to $1^{q}0(-1)^{n-q-1}$. Then, $b^{q}1^{q}0(-1)^{n-q-1}c^{n-q-1}$ is row j in $M^2(A, B, C)$ and it must be of the form $1^r0^s(-1)^t$ for some $r, s, t \ge 0$. So, we obtain $b = 1^n$ and $c^n = (-1)^n$ and $1^{nq+q}0(-1)^{n^2-nq-q-1}$ is a row of $M^2(A, B, C)$. Note that $B^q C^{n-q}$ is m consecutive rows of M^2 obtained by applying the morphism to $1^q(-1)^{n-q}$, and $1^{nq}(-1)^{n(n-q)}$ is row j in $B^q C^{n-q}$. Since $1^{nq+q}0(-1)^{n^2-nq-q-1}$ and $1^{nq}(-1)^{n(n-q)}$ are rows in $M^2(A, B, C)$, the conditions of Theorem 69 are not satisfied for $M^2(A, B, C)$. So, $M^2(A, B, C)$ is not semi-transitive, which is a contradiction. By the same argument, we also obtain a contradiction in the case of $1^{q-1}0(-1)^{n-q} \notin R(A)$. Hence $1^q(-1)^{n-q}$ cannot be a row in A.

Suppose that $1^{p}0(-1)^{n-p-1}$ is row *i* in *A*. By Theorem 69, we have that 1^{n} and $(-1)^{n}$ are not rows in $M^{1}(A, B, C)$. By Lemma 92, we have that 01^{n-1} , $1^{n-1}0$, $0(-1)^{n-1}$ and $(-1)^{n-1}0$ are not rows in $M^{1}(A, B, C)$. If there is a row in *A* of the form $1^{u}0(-1)^{n-u-1}$, where $1 \le u \le n-2$, by (5) in Lemma 91, we have p = u.

Hence, we obtain

$$A = \begin{bmatrix} 1^{p} & 0 & (-1)^{n-p-1} \\ 1^{p} & 0 & (-1)^{n-p-1} \\ \vdots & \vdots & \vdots \\ 1^{p} & 0 & (-1)^{n-p-1} \end{bmatrix} \text{ where } 1 \le p < n-2.$$

Let b and c be row j in B and C, respectively, for any $1 \leq j \leq m$. Note that B^pAC^{n-p-1} is m consecutive rows of M^2 obtained by applying the morphism to $1^{p}0(-1)^{n-p-1}$. Then, $b^{p}1^{p}0(-1)^{n-p-1}c^{n-p-1}$ is row j in $M^2(A, B, C)$ and it must be of the form $1^r0^s(-1)^t$ for some $r, s, t \geq 0$. So, we obtain $b = 1^n$ and $c = (-1)^n$. Hence, we see that B and C are all 1 matrix and all (-1) matrix, respectively.

Assume that $1^{p}0(-1)^{n-p-1}$ is not a row in A for any $1 \le p \le n-2$. That is, every row in A is 01^{n-1} , $1^{n-1}0$, 1^{n} , $0(-1)^{n-1}$, $(-1)^{n-1}0$ or $(-1)^{n}$. By Lemma 91, we need to consider the following two cases.

Case 1: $01^{n-1}, 0(-1)^{n-1} \in R(A)$ and $1^{n-1}0, (-1)^{n-1}0 \notin R(A)$. That is, every row in A is $01^{n-1}, 1^n, 0(-1)^{n-1}$ or $(-1)^n$. Suppose that 01^{n-1} is a row in A. Then, AB^{n-1} is m consecutive rows in $M^2(A, B, C)$. Let row i in B be b. Consider the following subcases:

- If row i in A is 01^{n-1} , then $01^{n-1}b^{n-1}$ is a row in $M^2(A, B, C)$. Since $b \neq 0^n$, we have $b = 1^n$.
- If row *i* in *A* is 1^n , then $1^n b^{n-1}$ is a row in $M^2(A, B, C)$. Since $b \neq 0^n$, we have $b = 1^n$.
- If row *i* in *A* is $0(-1)^{n-1}$, then $0(-1)^{n-1}b^{n-1}$ is a row in $M^2(A, B, C)$. Since $b \neq 0^n$, we have $b = (-1)^n$.

• If row i in A is $(-1)^n$, then $(-1)^n b^{n-1}$ is a row in $M^2(A, B, C)$. Since $b \neq 0^n$, we have $b = (-1)^n$.

Suppose that $0(-1)^{n-1}$ is a row in A. Then, AC^{n-1} is m consecutive rows in $M^2(A, B, C)$. Let row i in C be c. Consider the following subcases:

- If row *i* in *A* is 01^{n-1} , then $0(-1)^{n-1}c^{n-1}$ is a row in $M^2(A, B, C)$. Since $c \neq 0^n$, we have $c = 1^n$.
- If row *i* in *A* is 1^n , then $1^n c^{n-1}$ is a row in $M^2(A, B, C)$. Since $c \neq 0^n$, we have $c = 1^n$.
- If row *i* in *A* is $0(-1)^{n-1}$, then $0(-1)^{n-1}c^{n-1}$ is a row in $M^2(A, B, C)$. Since $c \neq 0^n$, we have $c = (-1)^n$.
- If row i in A is $(-1)^n$, then $(-1)^n c^{n-1}$ is a row in $M^2(A, B, C)$. Since $c \neq 0^n$, we have $c = (-1)^n$.

Thus, we see that (A, B, C) is left-0-invariant.

Case 2: $1^{n-1}0, (-1)^{n-1}0 \in R(A)$ and $01^{n-1}, 0(-1)^{n-1} \notin R(A)$. With the same way of the case 1, we can prove that (A, B, C) is right-0-invariant.

Thus, " \Rightarrow " has been proved. Lemma 96 gives us the converse.

3.3 Concluding remarks

In this chapter, we fully classified semi-transitivity of infinite families of directed split graphs generated by iterations of morphisms in the cases when the matrix A

has a 0. This research is a first step towards a classification of semi-transitive directed graphs in terms of positions of 0s and 1s (and (-1)s in the lower-triangular case) in the adjacency matrices. An application of such a classification could be in finding more efficient algorithms to recognize semi-transitivity of a directed graph, which is a problem solvable in polynomial time [KL15]. More importantly, a classification of semi-transitive directed graphs via adjacency matrices may lead to a better understanding of which (undirected) graphs admit semi-transitive orientations; this is an NP-complete problem [Kit17, KL15]. Should the general problem resist attempts to solve it, one could shift their attention to classification of semitransitivity of naturally defined (infinite) families of directed graphs. Such a shift should allow discovering new methods to deal with semi-transitivity of oriented graphs, and hence bring us closer to solving the general problem.

For yet another direction of research, note that Definition 77 of the index of semi-transitivity IST(A, B, C) makes sense in many situations when A has no 0's. For example, if A, B and C contain only 1's, we still can apply Definition 77 to see that IST $(A, B, C) = \infty$. On the other hand, Definition 77 does not work, for example, in the case when A is any matrix without 0's while B and C contain only 0's, as the infinite graph $G_o(A, B, C)$ is then not well-defined. Indeed, in the later case we see that $G_o^i(A, B, C)$ is not an induced subgraph of $G_o^{i+1}(A, B, C)$ while $G_o^i(A, B, C)$ is an induced subgraph of $G_o^{i+2}(A, B, C)$ for any $i \ge 0$, so that we have two infinite chains of induced subgraphs leading to two different infinite graphs as the limits (one of which is with no edges between the clique and the independent set). For another example, letting A be an all one matrix, B be an all (-1) matrix, and C be an all zero matrix, we witness the situation of three infinite chains of induced subgraphs with three infinite graphs as the limits. In any case, the problem we solved in this chapter can be extended to the case of matrices A with no 0's in the situations when the limiting infinite graph is uniquely defined, and the goal then is to classify such triples (A, B, C) with $IST(A, B, C) = \infty$. Of course, extra care should be taken about Definition 37 as it still may not work. For example, A without 0's can easily be chosen so that $G_0^1(A, B, C)$ has directed cycles and thus is not semi-transitive, while then choosing B and C be all one matrices, we see that $G_0^k(A, B, C)$ is semi-transitive for k > 1, so that the limiting graph is also semi-transitive and it is natural to assume that $IST(A, B, C) = \infty$, while by Definition 37, IST(A, B, C) = 1. However, natural adjustments to Definition 37 could be introduced. For example, we can define $IST(A, B, C) := \infty$ if there exists a natural number k such that $G_o^i(A, B, C)$ is semi-transitive for every $i \ge k$.

Part II

Encoding Labelled *p*-Riordan Graphs by Words and Pattern-avoiding Permutations

Chapter 4

Encoding Labelled *p*-Riordan Graphs by Words and Pattern-avoiding Permutations

This chapter, based on [IJK21], presents encoding *p*-Riordan graphs by *p*-Riordan words. Then we consider encoding Riordan graphs by pattern-avoiding permutations. After that, we encode oriented Riordan graphs by balanced words over the alphabet $\{0, 1, 2\}$, and provide, as a bi-product, a proof of a known enumerative result related to the formula (1.4).

4.1 Encoding *p*-Riordan graphs by *p*-Riordan words

Firstly, we define the following set of words that we call p-Riordan words because they will be proved by us in this section to be in 1-to-1 correspondence with pRiordan graphs.

Definition 98. A p-Riordan word $w_1w_2\cdots w_n$, $n \ge 1$, is a word over the alphabet $A^{(p)} = \{a_{i,j} : 0 \le i, j \le p-1\}$ such that either it is $a_{0,0}a_{0,0}\cdots a_{0,0}$ or there exist i and b, $1 \le i \le n, 1 \le b \le p-1$, such that the prefix $w_1\cdots w_i = a_{0,0}a_{0,0}\cdots a_{0,0}a_{b,0}$.

By definition, the empty word ε is a *p*-Riordan word of length 0. The set of *p*-Riordan words of length *n* is denoted by $\mathcal{W}_n^{(p)}$. For example, letting $a = a_{0,0}$, $b = a_{1,0}$, $c = a_{0,1}$ and $d = a_{1,1}$, then

$$\mathcal{W}_{3}^{(2)} = \{aaa, aab, aba, abb, abc, abd, baa, bab, bac, bad, bba, bbb, bbc, bbd, bca, bcb, bcc, bcd, bda, bdb, bdc, bdd\}.$$

Recall that $\mathcal{RG}_n^{(p)}$ is set of *p*-Riordan graphs with *n* vertices, and $\mathcal{W}_n^{(p)}$ is the set of *p*-Riordan words of length *n* (which is defined in Definition 98). In this section, we will present a bijective map $\xi : \mathcal{RG}_{n+1}^{(p)} \to \mathcal{W}_n^{(p)}$ for $n \ge 0$ and discuss its applications in the case of Riordan graphs (the case p = 2).

Theorem 99. There is bijection between $\mathcal{RG}_{n+1}^{(p)}$ and $\mathcal{W}_n^{(p)}$.

Proof. By definition, a p-Riordan graph $G = G_n^{(p)}(g, f)$ of order n can be determined by the coefficients $g_{b^*}, g_{b^*+1}, \ldots, g_{n-2}, f_1, f_2, \ldots, f_{n-b^*-2}$ where b^* is the smallest $i \in \{0, 1, \ldots, n-2\}$ such that $g_i \neq 0$; if no such i exists then G is an empty graph (a graph with no edges). Thus, $G_n^{(p)}(g, f) = G_n^{(p)}(\tilde{g}, \tilde{f})$ where \tilde{g} and \tilde{f} are the following polynomials:

•
$$\tilde{g} := \sum_{i=b^*}^{n-2} g_i t^i$$
 and $\tilde{f} := \sum_{i=1}^{n-2-b^*} f_i t^i$ if b^* is defined;

• $\tilde{g} = \tilde{f} = 0$ if b^* does not exist.
If $s_n^{(p)} = |\mathcal{W}_n^{(p)}|$ then $s_1^{(p)} = p$ and

$$s_{n+1}^{(p)} = p^2(s_n^{(p)} - 1) + p.$$
(4.1)

Indeed, $\mathcal{W}_{1}^{(p)} = \{a_{0,i} : 0 \leq i \leq p-1\}$ and to generate all elements in $\mathcal{W}_{n+1}^{(p)}$ we can extend every word in $\mathcal{W}_{n}^{(p)}$ different from $a_{0,0} \cdots a_{0,0}$ by any letter in $A^{(p)}$ (which explains the term $p^{2}(s_{n}^{(p)}-1)$), and the remaining p elements in $\mathcal{W}_{n+1}^{(p)}$ are given by $\{a_{0,0} \cdots a_{0,0} a_{b,0} : 0 \leq b \leq p-1\}$.

We note that $r_n^{(p)}$ satisfies the same recursion as (4.1), namely,

$$r_{n+1}^{(p)} = p^2 (r_n^{(p)} - 1) + p \tag{4.2}$$

with the initial condition $r_2^{(p)} = p$, which provides an alternative proof of (1.3). Indeed, the initial condition counts the p graphs on 2 vertices given by $\tilde{g}_0 = i$, $0 \le i \le p-1$. Also, to generate all graphs in $\mathcal{RG}_{n+1}^{(p)}$, we can take any non-empty graph in $\mathcal{RG}_n^{(p)}$ given by $\tilde{g} \ne 0$ and \tilde{f} , and choose independently g_{n-1} and f_{n-b^*-1} in $\{0, 1, \ldots, p-1\}$ (b^* is defined). This explains the term " $p^2(r_n^{(p)}-1)$ " in (4.2). The only uncounted graphs in $\mathcal{RG}_{n+1}^{(p)}$ are those given by $\tilde{g} = it^{n-1}$ where $0 \le i \le p-1$, which explains the term "+p".

For the only graph on one vertex, $\xi(G_1^{(p)}(0,0)) = \varepsilon$, and for $n \ge 2$, $\xi(G_n^{(p)}(g,f))$ is defined by

$$a_{g_0,f_{n-2}}a_{g_1,f_{n-3}}\cdots a_{g_{b^*-1},f_{n-3-b^*}}a_{g_{b^*},f_0}a_{g_{b^*+1},f_1}a_{g_{b^*+2},f_2}\cdots a_{g_{n-2},f_{n-2-b^*}} = a_{0,0}a_{0,0}\cdots a_{0,0}a_{1,0}a_{g_{b^*+1},f_1}a_{g_{b^*+2},f_2}\cdots a_{g_{n-2},f_{n-2-b^*}}$$

where $g_i = [t^i]\tilde{g}$ and $f_j = [t^j]\tilde{f}$. The fact that ξ is well-defined and bijective essentially follows from our proofs of (4.1) and (4.2).

The bijection ξ given in Theorem 99 allows us to encode by words three classes of Riordan graphs (the case p = 2). As above, we let $\mathcal{W}_n^{(2)}$ be words over $\{a, b, c, d\}$, where $a = a_{0,0}$, $b = a_{1,0}$, $c = a_{0,1}$ and $d = a_{1,1}$, Justifications of our encodings are straightforward from the properties of ξ .

The class (1 + f, f). In this case, g = 1 + f. Since $[t^0]g = 1$ and $[t^i]g = [t^i]f$ for each $i \in [n-2]$, we have that $b^* = 0$ and the words in $\mathcal{W}_n^{(2)}$ corresponding to these graphs are those of the form $bx_1x_2\cdots x_{n-1}$ where $x_i \in \{a, d\}$.

Proper Riordan graphs. For a proper Riordan graph $g_0 = f_1 = 1$, so $b^* = 0$ and the words in $\mathcal{W}_n^{(2)}$ corresponding to these graphs are those beginning either with *bc* or with *bd* for $n \ge 2$, and $\mathcal{W}_1^{(2)} = \{b\}$.

Riordan graphs of the Appel type. For these graphs f = t, and thus the words in $\mathcal{W}_n^{(2)}$ corresponding to these graphs are of the form $aa \cdots a$, $aa \cdots ab$ and $aa \cdots abxw$ for $x \in \{c, d\}$ and w a word over the alphabet $\{a, b\}$.

4.2 Encoding Riordan graphs by

pattern-avoiding permutations

The sequence $(r_n)_{n\geq 0}$ counting Riordan graphs and given by (1.2) has various combinatorial interpretations recorded in A047849 in the *On-Line Encyclopedia* of Integer Sequences (OEIS) [Slo]. Two of these interpretations are related to pattern-avoiding permutations:

(I1) r_n counts permutations in $S_{2n}(123, 132)$ with two fixed points; the set of such permutations is denoted by P_{2n} ; see [MR02].



Figure 4.1: The structure of a permutation in P_{2n}

(I2) r_n counts permutations in $S_n(4321, 4123)$, or in $S_n(4321, 3412)$, or in $S_n(4123, 3214)$, or in $S_n(4123, 2143)$; see [KS03].

In this section, we explain combinatorially a connection between Riordan graphs and (I1). Moreover, we will show which permutations, under the bijection we will construct, correspond to Riordan graphs of the Appell type, of the Bell type (including the Pascal graph), of the derivative type, as well as of the types given by (1+f, f) and (g, 0) (a star graph with a number of isolated vertices), and to proper Riordan graphs. We leave explaining the second bullet point combinatorially as an open problem.

Theorem 100. There is a bijection between \mathcal{RG}_n and P_{2n} .

Proof. Let $\pi = p_1 p_2 \cdots p_{2n}$ and a and b be the two fixed points in π where $1 \leq a < b \leq 2n$. Since π avoids the patterns 123 and 132, the remaining 2n - 2 elements can only be placed in the areas A, B, C and D in Figure 4.1, where we show π schematically as a permutation diagram. In addition, the elements in B and C must be in decreasing order, while A (resp., D) avoids 123 and 132, and is

independent from the rest of π in the sense that no occurrence of 123 or 132 can start in A (resp., D) and end elsewhere. Since the number of elements in B and C is b - a - 1, we obtain that the number of elements in D, which is the same as the number of elements in A, is

$$2n - b = a - 1 - (b - a - 1) \quad \Rightarrow \quad a = n.$$

Thus, B and C have the same number of elements b - n - 1, and π satisfies

- $p_1p_2\cdots p_{2n-b}$ and $p_{b+1}p_{b+2}\cdots p_{2n}$ avoid the patterns 123 and 132;
- $p_{2n-b+i} = b i$ for each $i = 1, 2, \dots, 2b 2n 1$.

The desired map $\phi : \mathcal{RG}_n \to P_{2n}$, is defined as follows where $\phi(G_n(g, f)) = p_1 p_2 \cdots p_{2n}$ and the function ψ is defined in Section 1.6:

- $p_n = n$ and $p_b = b$ where $b = b^* + n + 1$ and $b^* = \min\{i \mid [t^i]g = 1\}$ if $g \neq 0$ and b = 2n if g = 0;
- $p_{2n-b+i} = b i$ for each $i \in [2b 2n 1];$
- $\psi(g_{b^*+1}g_{b^*+2}\cdots g_{n-2}) = (p_1-b)\cdots(p_{2n-b}-b)$ so that to obtain $p_1\cdots p_{2n-b}$ we apply ψ to $g_{b^*+1}g_{b^*+2}\cdots g_{n-2}$ and then increase each element in the obtained permutation by b (lengths are proper here since $b = b^* + n + 1$);
- $\psi(f_1 f_2 \cdots f_{2n-b-1}) = p_{b+1} \cdots p_{2n}$.

It is not difficult to see that ϕ is well-defined and injective. Thus, since $|\mathcal{RG}_n| = |P_{2n}|, \phi$ is bijective. For example, $\phi(G_5(t+t^3,t^2)) = (10)896547312$ and $\phi(G_5(t,t+t^2)) = 98(10)6547321$. In particular, in both cases n = 5, 2n = 10 and $b^* = 1$ so that b = 7.

The bijection ϕ given in Theorem 100 allows us to describe subclasses of Riordan graphs in terms of pattern-avoiding permutations. In our description we refer to A and D to be the parts of a permutation $\pi = p_1 \cdots p_{2n}$ schematically given in Figure 4.1. That is, $A = p_1 \cdots p_{2n-b}$ and $D = p_{b+1} \cdots p_{2n}$. Justifications of our descriptions are usually straightforward from the properties of ϕ , but in some places we still provide various clarifications. In what follows recall that $b = b^* + n + 1$.

The class (1 + f, f). In this case, g = 1 + f. Since $[t^0]g = 1$ and $[t^i]g = [t^i]f$ for each $i \in [n-2]$, we have that $b^* = 0$ and the permutations in P_{2n} corresponding to these graphs have the fixed points n and n + 1, and red(A) = D.

Proper Riordan graphs. For a proper Riordan graph $g_0 = f_1 = 1$, so $b^* = 0$ and the permutations in P_{2n} corresponding to these graphs have two fixed points n and n + 1, and the minimal element in D is in the last place.

Riordan graphs of the Appel type. For these graphs f = t and thus the permutations in P_{2n} describing them are those for which $D = (2n - b - 1)(2n - b - 2) \cdots 32(2n - b)1$.

Riordan graphs of the Bell type. Such graphs are given by (g, tg) where either g = 0 or $g_0 = g_1 = \cdots = g_{b^*-1} = 0$ and $g_{b^*} = 1$ for $b^* \ge 0$. In the former case, we deal with the empty graph corresponding to $(2n-1)(2n-2)\cdots 1(2n)$. For the latter case, since $\tilde{f} = g_0 t + g_1 t^2 + \cdots + g_{n-2-b^*} t^{n-1-b^*}$, we can conclude that permutations in P_{2n} corresponding to the Riordan graphs of the Bell type are those having the

 $b^* + 1$ rightmost elements of D forming the permutation $b^*(b^* - 1) \cdots 21(b^* + 1)$. We note that the Pascal graph $\left(\frac{1}{1-z}, \frac{z}{1-z}\right)$ is the only graph of the Bell type that belongs to the class (1 + f, f). For this graph $b^* = 0$, b = n + 1, and the permutation in P_{2n} corresponding to it is $(2n)(2n-1)\cdots(n+2)n(n+1)(n-1)(n-2)\cdots 1$.

Riordan graphs of the derivative type. This class of graphs is of the form (f', f) so $g = f' = f_1 + f_3 t^2 + f_5 t^4 + \cdots$. Thus, permutations corresponding to such graphs can be described algorithmically by imposing the following restrictions on A: in implementing the bijection ψ every even step must place the current element into the left out of two valid slots. Thus, if this rule is not violated, the obtained permutation corresponds to a Riordan graph of the derivative type.

4.3 Encoding oriented Riordan graphs by balanced words over {0,1,2}

The sequence \tilde{r}_n counting oriented Riordan graphs $\mathcal{RG}_n^{(3)}$ and given by (1.4) is A054879 in [Slo], one of whose interpretations is the number of words of length 2n on alphabet $\{0, 1, 2\}$ with an even number (possibly zero) of each letter. We call these words *balanced words* and denote the respective set by \mathcal{B}_n . Also, let $b_n := |\mathcal{B}_n|$. The words in \mathcal{B}_n are clearly in 1-to-1 correspondence with closed walks of length 2n along the edges of the 3-cube (cube) starting at the origin. Such walks also mentioned in A054879. The correspondence is given by letting a walk take the *i*-th step in direction $x, 1 \leq x \leq 3$ (that is, swap the *i*-th coordinate from 0 to 1, or vice versa) in the case if the *i*-th letter in the word is x - 1. The formula for b_n (the same as (1.4)) is given in A054879 in [Slo], but its derivation would involve simplifying a more general result in [Rey]

$$\frac{1}{2^n}\sum_{j=0}^n \binom{n}{j}(n-2j)^r$$

after placing n = 3 there. As a bi-product, in this section we obtain an alternative justification of (1.4) be valid for b_n after explaining combinatorially the recursion (4.4).

To build a recursive encoding in question, we will use an alternative, inductive way to prove formula (1.4) via first explaining combinatorially the recursion

$$\tilde{r}_{n+1} = 3\tilde{r}_n + 6(\tilde{r}_n - 1), \tag{4.3}$$

which is a particular case of p = 3 in (4.2) proved above. Next, we explain

$$b_{n+1} = 3b_n + 6(b_n - 1), (4.4)$$

which, again, will provide an alternative proof for the formula (1.4) for b_n given in A054879.

Explanation of (4.3). Each graph $G_{n+1}(g, f)$ in $\mathcal{RG}_{n+1}^{(3)}$ either has

- $f_{n-b^*-1} = 0$ (in the case b^* is not defined we can assume $\tilde{f} = 0$), and there are $3\tilde{r}_n$ ways to select such G, where "3" is the number of choices for g_{n-1} , or
- $f_{n-b^*-1} \in \{1,2\}$ and $g_0g_1 \dots g_{n-2} \neq 00 \dots 0$, so that there are 3 choices for g_{n-1} and in total $6(b_n-1)$ ways to select such a G.

This completes the proof of (4.3).

Explanation of (4.4). We note that any balanced word either ends with xx or with $xy, x \neq y, x, y \in \{0, 1, 2\}$. Clearly, there are $3b_n$ words in \mathcal{B}_{n+1} ending with 00 or 11 or 22. Next, we prove that there are $6(b_n - 1)$ words in \mathcal{B}_{n+1} ending with $xy, x \neq y$. To generate any such word we use the function $h_{x,y}$ that

- takes any word w in \mathcal{B}_n different from $zz \cdots z$ for $z \neq x, y$, then
- replaces the leftmost occurrence of an element in {x, y} in w by the opposite from the same set, and
- attaches xy to the obtained word.

For example, for x = 0 and y = 1, $h_{0,1}(22012120) = 2211212001$. Note that $h_{x,y}$ is well-defined because its outcome is a balanced word.

Next note that $h_{x,y}$ is injective. Indeed, different words, say w_1 and w_2 , would either get different endings, and thus will result in different outcomes, or they will have the same ending. In the later case, if such an ending is xx then we clearly have different outcomes. Otherwise, the ending is xy for $x \neq y$. Consider the smallest $i \geq 1$ such that the *i*-th element in w_1 is different from the *i*-th element in w_2 (such an *i* exists). Thus, $w_1 = x_1x_2\cdots x_{i-1}a\cdots$ and $w_2 = x_1x_2\cdots x_{i-1}b\cdots$ and $a \neq b$. If none of the *a* and *b* would be changed by $h_{x,y}$, the outcome words are different. On the other hand if, without loss of generality *a* will be changed, then $x_1x_2\cdots x_{i-1} = zz\cdots z$ for $z \neq x, y$, and thus either

- b = z in which case we obtain $h_{x,y}(w_1) \neq h_{x,y}(w_2)$ as $a \neq z$, or
- b in w₂ will be changed as well, so that h_{x,y}(w₁) and h_{x,y}(w₂) differ in position
 i.

So, in either case, $h_{x,y}(w_1) \neq h_{x,y}(w_2)$.

We finally prove surjectivity of $h_{x,y}$ that completes our proof of (4.4). Given a word $w_1w_2\cdots w_{2n+2} \in \mathcal{B}_{n+1}$ we replace the leftmost occurrence of a letter in $\{w_{2n+1}w_{2n+2}\}$ in $w_1w_2\cdots w_{2n}$ by the opposite from the same set so that the resulting word belongs to \mathcal{B}_n . For example, $h_{x,y}^{-1}(0021210202) = 20212102$.

Theorem 101. There is a bijection between $\mathcal{RG}_{n+1}^{(3)}$ and \mathcal{B}_n .

Proof. We describe recursively a bijective map $\eta : \mathcal{RG}_{n+1}^{(3)} \to \mathcal{B}_n$ based on our proofs of relations (4.3) and (4.4) with the base cases $\eta(G_2(0,0)) = 00, \eta(G_2(1,0)) =$ 11 and $\eta(G_2(2,0)) = 22$.

Suppose that η is already defined for $\mathcal{RG}_n^{(3)}$, $n \ge 2$, and $\eta(G_n(g, f)) = w_1 w_2 \cdots w_{2n-2}$. Moreover, we make the following assumptions, which work for the base case and will work for n + 1 as well:

- $\eta(G_n(0,0)) = 00 \cdots 0;$
- $\eta(G_n(1+t+\cdots+t^{n-2},0)) = 11\cdots 1;$
- $\eta(G_n(2+2t+\cdots+2t^{n-2},0))=22\cdots 2.$

Then, adding g_{n-1} and f_{n-b^*-1} into consideration results in a graph $G \in \mathcal{RG}_{n+1}^{(3)}$ obtained from $G_n(g, f)$ by adding one vertex, and we define $\eta(G)$ by the following rules:

- If $f_{n-b^*-1} = 0$ or $\tilde{f} = 0$ (in the case b^* is not defined) then $\eta(G) = w_1 w_2 \cdots w_{2n-2} g_{n-1} g_{n-1}$.
- If $f_{n-b^*-1} = 1$, then we can take any $G_n(g, f)$ except for the one with $\tilde{g} = 0$ corresponding to $w_1w_2\cdots w_{2n-2} = 00\cdots 0$, and consider the following subcases:

- if $g_{n-1} = 0$ then $\eta(G) = h(w_1w_2\cdots w_{2n-2})01$ if $w_1w_2\cdots w_{2n-2} \neq 22\cdots 2$ and $\eta(G) = h(00\cdots 0)01 = 100\cdots 01$ otherwise; note that this rule is injective, well-defined for any $G_n(g, f)$ different from an empty graph, and covers all words in \mathcal{B}_n ending with 01.
- if $g_{n-1} = 1$ then $\eta(G) = h(w_1 w_2 \cdots w_{2n-2}) 12$, which is well-defined since $w_1 w_2 \cdots w_{2n-2} \neq 00 \cdots 0$, injective, and covers all words in \mathcal{B}_n ending with 12.
- if $g_{n-1} = 2$ then $\eta(G) = h(w_1w_2\cdots w_{2n-2})02$ if $w_1w_2\cdots w_{2n-2} \neq 11\cdots 1$ and $\eta(G) = h(00\cdots 0)02 = 200\cdots 02$ otherwise; note that this rule is injective, well-defined for any $G_n(g, f)$ different from an empty graph, and covers all words in \mathcal{B}_n ending with 02.
- If $f_{n-b^*-1} = 2$, then we can take any $G_n(g, f)$ except for the one with $\tilde{g} = 0$ corresponding to $w_1 w_2 \cdots w_{2n-2} = 00 \cdots 0$, and consider the following subcases:
 - if $g_{n-1} = 0$ then $\eta(G) = h(w_1w_2\cdots w_{2n-2})10$ if $w_1w_2\cdots w_{2n-2} \neq 22\cdots 2$ and $\eta(G) = h(00\cdots 0)10 = 100\cdots 010$ otherwise; note that this rule is injective, well-defined for any $G_n(g, f)$ different from an empty graph, and covers all words in \mathcal{B}_n ending with 10.
 - if $g_{n-1} = 1$ then $\eta(G) = h(w_1 w_2 \cdots w_{2n-2}) 21$, which is well-defined since $w_1 w_2 \cdots w_{2n-2} \neq 00 \cdots 0$, injective, and covers all words in \mathcal{B}_n ending with 21.
 - if $g_{n-1} = 2$ then $\eta(G) = h(w_1 w_2 \cdots w_{2n-2}) 20$ if $w_1 w_2 \cdots w_{2n-2} \neq 11 \cdots 1$ and $\eta(G) = h(00 \cdots 0) 20 = 200 \cdots 020$ otherwise; note that this rule is

injective, well-defined for any $G_n(g, f)$ different from an empty graph, and covers all words in \mathcal{B}_n ending with 020.

The fact that η is well-defined and bijective follows from our remarks above. For example, $w = \eta(G_5(1 + 2t^2 + t^3, t^2))$ can be recursively calculated from $\eta(G_4(1 + 2t^2 + t^3, t^2))$ and $g_{n-1} = g_4 = 0$ and $f_{n-b^*-1} = f_{5-1-1} = f_3 = 0$ so that w will end with 00. In turn, $w' = \eta(G_4(1 + 2t^2 + t^3, t^2))$ can be recursively calculated from $\eta(G_3(1 + 2t^2 + t^3, t^2))$ and $g_3 = 1$ and $f_2 = 1$, so that w' will end with 12. And so on. One can check that w = 2100221200.

4.4 Concluding remarks

This chapter provides a convenient encoding of *p*-Riordan graphs in terms of *p*-Riordan words, and explains combinatorially some links between (oriented) Riordan graphs and balanced words (equivalently, certain closed walks in a cube) and pattern-avoiding permutations.

We leave it as an open question to explain combinatorially that the sequence $(r_n)_{n\geq 0}$ counting Riordan graphs and given by (1.2) also counts permutations in $S_n(4321, 4123)$, or in $S_n(4321, 3412)$, or in $S_n(4123, 3214)$, or in $S_n(4123, 2143)$ that were enumerated in [KS03]; also see A047849 in [Slo]. A natural approach would be to use 2-Riordan words that are in bijection with Riordan graphs to establish a correspondence in question. However, enumeration of pattern-avoiding permutations in [KS03] is rather involved (it uses the notion of an *active site*) and e.g. cannot be translated that easily into recursion (4.1) for p = 2.

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