

Valid Path Numberings in Circulant Graphs

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ABSTRACT

Assigning labels to the vertices and/or edges of a given graph $G = (V, E)$, respecting predefined conditions, is a well-known research problem in the field of Graph Theory. The labelling of a graph G , of order n , is defined as a *numbering* when the set of integers $\{1, \dots, n\}$ is used to label $V(G)$ in a distinct way. A path with three vertices is termed *valid* if the label associated with its central vertex is smaller than the labels associated with the endpoints of the path. The *Valid Paths Problem* involves finding a numbering that optimises the number of valid paths in G . The focus of this work is on the class of *circulant graphs* and, in particular, two sub-classes called *prefix circulant graphs* and *suffix circulant graphs*, for which a particular numbering π^I is defined. The quantity of valid paths induced by π^I is proved to be minimum in *prefix circulant graphs* and maximum in *suffix circulant graphs*. An algorithm to perform such a numbering in arbitrary graphs is also proposed.

KEYWORDS. Numbering, circulant graph, 2-path, valid path, power of cycle.

RESUMO

A atribuição de rótulos aos vértices e/ou arestas de um dado grafo $G = (V, E)$, respeitando-se condições pré-definidas, é um problema bem conhecido da área de Teoria de Grafos. A rotulagem de um grafo G , de ordem n , é definida como numeração quando o conjunto de inteiros $\{1, \dots, n\}$ é usado para rotular $V(G)$ de maneira distinta. Um caminho com três vértices é considerado válido se o rótulo associado ao seu vértice central for menor que os rótulos associados aos vértices nos extremos do caminho. O *Problema dos Caminhos Válidos* envolve encontrar uma numeração que otimize o número de caminhos válidos em G . O foco deste trabalho é a classe de *grafos girculantes* e, em particular, duas subclasses denominadas *grafos circulantes prefixais* e *grafos circulantes sufixais*, para as quais são definidas uma numeração específica π^I e a quantidade de caminhos válidos induzidos por π^I . A quantidade de caminhos válidos induzida por π^I é provada ser mínima em *grafos circulantes prefixais* e máxima em *grafos circulantes sufixais*. Um algoritmo para realizar tal numeração em grafos de quaisquer classes também é proposto.

PALAVRAS CHAVE. Numeração, grafo circulante, bicaminho, caminho válido, potência de ciclo.

1. Introduction

Graph Theory is the study of graphs, which are mathematical structures used to model pairwise relations among objects. One sub-field of Graph Theory is *graph labelling*, which was first introduced in the seminal paper by Rosa [1967]. A labelling of a graph is an assignment of labels to its vertex or edge sets (or both), subject to certain conditions. After Rosa's article, thousands of studies have been published and until 2021, many of them were listed in Gallian's survey [Gallian, 2021], which was updated for 25 years. Usually the term *graph labelling* is related to vertex labelling and this is done in the present article.

Several well-known optimisation problems on graphs can be formulated in terms of labelling as follows: given a graph G , find a labelling of G such that a given linear function of the chosen labelling is optimised. Applications fields include, among others, network addressing [Judd and Beer, 1995], circuit layout code design [Shieh et al., 2011] and the bandwidth, minimum-sum and cutwidth problems [Chung, 1981; Juvan and Mohar, 1992]. Some problems in this field are also related to defining some ordering of the vertices of G and applying some given set of operations based on this order. When G is of order n (i.e. has n vertices), this kind of labelling can be formally defined as a *vertex numbering*, where each vertex is labelled with a distinct number from the set $[n] = \{1, \dots, n\}$. Such a labelling can also be seen as a permutation of the vertices of G .

Bloom and Golomb [1977] showed that vertex numbering has a wide range of applications, most of them based on mathematical models, such as the analysis of various coding theory problems, including the design of good radar-type codes, sync-set and convolutional codes with optimal auto-correlation properties. They also mentioned applications to problems in additive number theory, the determination of ambiguities in X-ray crystallographic analysis, the design of communication network addressing systems and the identification of optimal circuit layouts.

Foulds and Longo [2023] introduced the concept of *Path Validity*, which is based on the vertex numbering of an arbitrary given graph G . A path in G is termed *valid* if it is a 2-path (a path with three vertices) and the number of the middle vertex label is smaller than the numbers of its endpoints. (Note that this concept is defined only for 2-paths.) The *Path Validity Problem* involves finding a numbering of a given graph G that optimises the quantity of valid paths in G induced by that numbering. This problem arises, for example, in the enumeration of chordless cycles in graphs, which has application in the prediction of nuclear magnetic resonance, chemical shift values and ecological networks [Dias et al., 2013].

The Path Validity Problem has only recently been proposed and, as far as we know, there are still no published studies about it in the open literature. This gap can be seen, for example, in the dynamic survey by Gallian [2021], considered by many researchers in this area to be the most complete survey of articles on graph labelling currently available. In the present work, vertex numbering is studied, focusing on defining numbering algorithm and on a specific class of graphs known as circulant graphs.

The remainder of the text is organized as follows. In Section 2, the definition of circulant graphs and some other related items are presented, based on the work of [Boesch and Tindell, 1984] and [Vilfred, 2017]. Section 3 formally defines the Path Validity Problem, based on the concepts introduced by [Foulds and Longo, 2023]. Section 4 describes an algorithm to determine a numbering that induces $\phi_{\min}(G)$ and $\phi_{\max}(G)$, (the minimum and maximum quantity of paths respectively), which is based on the dynamic programming technique. Next, some results and definitions related to the maximal and minimal number of valid paths in circulant graphs are given in Section 5. Section 6 rounds out the paper with a conclusion, some suggestions for future work and some conjectures.

2. Circulant graphs

A *circulant matrix* of order n is a square matrix of the form:

$$C = \text{circ}(c_1, c_2, \dots, c_n) = \begin{bmatrix} c_1 & c_2 & \cdots & c_n \\ c_n & c_1 & \cdots & c_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_2 & c_3 & \cdots & c_1 \end{bmatrix} \quad (1)$$

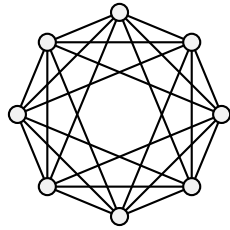
The elements of each row of C are identical to those of the previous row, but are moved one position to the right. The whole circulant matrix is determined by the first row.

A *binary circulant matrix* is a matrix, such that the elements in each position of the matrix is either 0 or 1 and they form a Circulant Matrix. An example is:

$$BC = \text{circ}(1, 1, 0, 1) = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}$$

Let $G = (V(G), E(G))$ be an undirected simple graph, with $n = |V(G)|$, $m = |E(G)|$ and B being the adjacency matrix of G . Given a vertex $v_1 \in V(G)$, the set $R = \{j - 1 \mid v_1 \in V(G), (v_1, v_j) \in E(G), j - 1 \leq \lfloor \frac{n}{2} \rfloor\}$ is the *connection set* of G if: (i) B is a binary circulant matrix; (ii) the first row of B is relative to vertex v_1 ; and (iii) B has 1's in columns $1 + j$ and $n + 1 - j$, such that $j \in R$ of the first row of B and 0's in the remaining ones.

A *Circulant graph* $C_n(R)$ is a graph with n vertices whose adjacency matrix B is a binary circulant matrix specified by a connection set R . Figure 1 illustrates a circulant graph with $n = 8$, $m = 24$, $R = \{1, 2, 3\}$ and its adjacency matrix B .



(a): $C_8(\{1, 2, 3\})$.

$$B = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \end{bmatrix}$$

(b): Adjacency matrix B of $C_8(\{1, 2, 3\})$.

Figure 1: Example of a circulant graph (a) and its adjacency matrix (b).

Given a circulant graph $C_n(R)$, the degree d of all its vertices is either $2|R|$, if $\frac{n}{2} \notin R$, or $2|R| - 1$, otherwise; where $|R|$ is the cardinality of the connection set R . In Figure 1, $\frac{n}{2} = \frac{8}{2} = 4 \notin R$ and thus $d = 2|R| = 2 \cdot 3 = 6$. Lemma 2.1, given next, states necessary and sufficient conditions for a circulant graph to be connected.

Lemma 2.1 ([Boesch and Tindell, 1984]) A circulant graph $C_n(R)$ for a set $R = \{r_1, r_2, \dots, r_k\}$ is connected if and only if $\gcd(n, r_1, r_2, \dots, r_k) = 1$.

Let R be connection set of a circulant graph G . If R is a *prefix contiguous subset*¹ of the set $\{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$, then G is a *prefix circulant graph*, denoted by $PC_n(R)$. If $|V(G)|$ is

¹ Given a set $E = \{e_1, e_2, \dots, e_n\}$, a *prefix contiguous subset* $P_k \subseteq E$ is the subset $P_k = \{e_1, e_2, \dots, e_k\}$, for $1 \leq k \leq n$; analogously, a *suffix contiguous subset* $S_k \subseteq E$ is the subset $S_k = \{e_k, e_{k+1}, \dots, e_n\}$, for $1 \leq k \leq n$.

even and R is a *suffix contiguous subset*¹ of the set $\{1, 2, \dots, \frac{n}{2}\}$, then G is a *suffix circulant graph*, denoted by $SC_n(R)$. We use the term *prefix circulant graphs* because it reflects the concepts arising in this article. The term is equivalent to the commonly used phrase *power of cycles*. Figures 2(a) and 2(b) illustrate two examples of prefix circulant graphs. Figures 2(c) and 2(d) illustrate two examples of suffix circulant graphs.

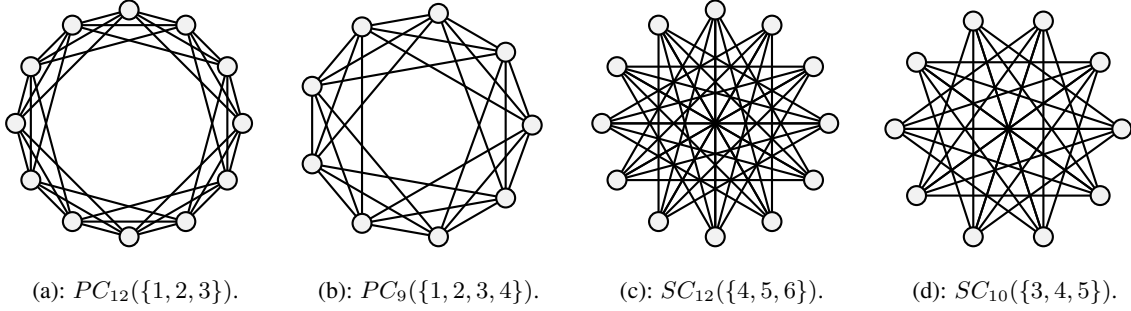


Figure 2: Examples of prefix and suffix circulant graphs.

3. The path validity problem

Given a graph $G = (V(G), E(G))$, a numbering π of G is a bijective mapping from $V(G)$ to $\{1, 2, \dots, n\}$ ($\pi(v)$ denotes the number associated with vertex $v \in V(G)$). If G has a such numbering, a 2-path $\langle x, u, y \rangle$ in G is said to be *valid* if the number associated with its middle vertex u is smaller than the numbers of its endpoints x and y , i.e., $\pi(u) < \min\{\pi(x), \pi(y)\}$. The squared adjacency matrix of G can be used to check if there is the possibility of a valid path existing between any given pair of vertices in $V(G)$.

The validity $\phi_\pi(G)$ of a numbering π of G is defined as the quantity of valid 2-paths of G induced by π , i.e.,

$$\phi_\pi(G) = |\{\langle x, u, y \rangle \mid u \in V(G), x, y \in \text{Adj}(u) \text{ and } \pi(u) < \min(\pi(x), \pi(y))\}|. \quad (2)$$

Given a vertex $u \in V(G)$ and a numbering π , the set of valid paths *induced by u in π* is the set of the valid paths in $\phi_\pi(G)$ such that each such path has u as its middle vertex. The *minimum validity* $\phi_{\min}(G)$ of G is the minimum of $\phi_\pi(G)$ over all numberings π , i.e.,

$$\phi_{\min}(G) = \min\{\phi_\pi(G) \mid \pi \text{ is a numbering of } G\}. \quad (3)$$

Analogously, the *maximum validity* $\phi_{\max}(G)$ of G is the maximum of $\phi_\pi(G)$, i.e.,

$$\phi_{\max}(G) = \max\{\phi_\pi(G) \mid \pi \text{ is a numbering of } G\}. \quad (4)$$

For general graphs, $\phi_{\min}(G)$ and $\phi_{\max}(G)$ can vary significantly, depending on the graph structure and how the numbering is carried out. If no constraints are imposed then $n!$ different numberings are possible, inducing sets of valid paths that may vary quite markedly. Figure 3 illustrates this phenomenon for three distinct numberings of the C_6 graph (the cycle with 6 vertices) with their valid paths indicated. The leftmost numbering is minimal as it induces only a single valid path, namely $\langle 2, 1, 6 \rangle$, and is a manifestation of $\phi_{\min}(C_6)$. The second numbering induces 2 valid paths, namely $\langle 4, 1, 5 \rangle$ and $\langle 3, 2, 5 \rangle$, and is neither minimal nor maximal. The rightmost numbering is maximal as it induces a triple of valid paths, namely $\langle 4, 1, 6 \rangle$, $\langle 4, 2, 5 \rangle$ and $\langle 5, 3, 6 \rangle$, and is a manifestation of $\phi_{\max}(C_6)$.

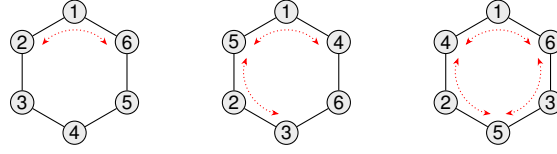


Figure 3: Three numberings of the C_6 graph.

As far as we know, finding numberings that achieve $\phi_{\min}(G)$ or $\phi_{\max}(G)$ for an arbitrary graph G are open problems, which are denoted by MIN-VP and MAX-VP, respectively, and are defined as:

Instance: A finite, undirected, simple graph G and a nonnegative integer k .

MIN-VP: Is there a numbering π of G that induces at most k valid paths in G , i.e., $\phi_{\pi}(G) \leq k$?

MAX-VP: Is there a numbering π of G that induces at least k valid paths in G , i.e., $\phi_{\pi}(G) \geq k$?

4. Algorithms

A simple brute force approach to finding both $\phi_{\min}(G)$ and $\phi_{\max}(G)$ for an arbitrary graph G involves enumerating all possible numberings of G , which takes $O(n!)$ time. We propose a much faster algorithm, even though it is still non-polynomial. This approach, which uses the dynamic programming technique, significantly reduces the number of possible combinations that need to be considered, eliminating those that cannot be part of an optimal solution to the enumeration problem, giving rise to a more efficient algorithm.

The basic idea of the improved approach is to iteratively construct an optimal solution stage by stage, by combining already obtained solutions for smaller, earlier stages. Thus, it is possible to choose sub-problems so that vital information is stored and carried forward.

Let $G = (V, E)$ be a graph of order n , where $V = \{v_1, v_2, \dots, v_n\}$. Suppose set $S \subseteq V$. Let $MinOpt(S)$ and $MaxOpt(S)$ be the minimum and maximum quantity, respectively, of valid paths obtained by labelling every vertex in S with a unique number in $\{1, \dots, |S|\}$. To achieve $MinOpt(S)$ and $MaxOpt(S)$, firstly a vertex $v \in S$ must be chosen and labelled as $|S|$. Thus, v induces valid paths for each pair of distinct vertices $u, u' \in S \setminus \{v\}$ such that $(u, v), (u', v) \in E$, leading to:

$$MinOpt(S) = \min_{v \in S} MinOpt(S \setminus \{v\}) + \sum_{\substack{u \in S \setminus \{v\}, \\ (u,v) \in E}} \sum_{\substack{u' \in S \setminus \{v,u\}, \\ (u',v) \in E}} 1; \quad (5)$$

$$MaxOpt(S) = \max_{v \in S} MaxOpt(S \setminus \{v\}) + \sum_{\substack{u \in S \setminus \{v\}, \\ (u,v) \in E}} \sum_{\substack{u' \in S \setminus \{v,u\}, \\ (u',v) \in E}} 1. \quad (6)$$

The *VertexCost* algorithm, whose pseudo-code is given as Algorithm 1, returns the quantity of valid paths induced by $v \in V(G)$, given that $\pi(v) = n - |S|$ and a subset $S \subset V(G) \setminus \{v\}$ is already numbered with a permutation of $\langle n - |S| + 1, \dots, n - 1, n \rangle$. Since all labels that are greater than $\pi(v)$ are already defined, it is only necessary to analyse the adjacencies between v and the vertices in S to determine the quantity of the valid paths induced by v .

Definition 4.1 Given a set S ,

$$\rho(S) = \bigcup_{x \in S} \{x\}$$

Algorithm 1: $VertexCost(v, S, G)$

Data: Graph $G = (V(G), E(G))$, vertex $v \in V(G)$, set S .

Result: Quantity of valid paths induced by v with label equal to $n - |S|$.

```

1  $qtd \leftarrow 0$ ;
2 foreach  $u \in V(G)$  do
3   if  $((v, u) \in E(G))$  and  $(u \in S)$  then
4      $qtd \leftarrow qtd + 1$ ;
5 return  $\binom{qtd}{2}$ .
```

Algorithm 1 assumes that every vertex $u \in S$ has a label greater than $n - |S|$. Thus, these vertices will all contribute to the quantity of valid paths induced by v . At Step 1 the variable qtd is initialised as 0. From Step 2 to Step 4, for each $u \in V(G)$, there is a check to see if there is an edge joining u and v and if u is in the set S . If u does indeed have these properties, the quantity is increased by one in Step 4. At Step 5 the quantity of valid paths induced by v is calculated and returned.

Algorithm 2 ($MinPath(G)$) returns the numbering that leads to the function $\phi_{\min}(G)$ of a given graph G . In Step 1 a Matrix DP with states for each subset of $[n] = \{1, \dots, n\}$ is created, initialised with ∞ in each position. In Step 2 to Step 5, S iterates through every subset of $[n]$ ordered by size. In Step 3 to Step 5, v iterates through every vertex of $V(G)$. In Step 4 it is verified if v is not in the set S . If $v \notin S$, v is tested with label $n - |S|$ (Step 5), increasing the quantity of induced valid paths by $VertexCost(v, S, G)$, updating the answer of $DP[S + \{v\}]$ with the minimum of the old value and the new value calculated as $DP[S] + VertexCost(v, S, G)$. At the end of Step 5 the minimum quantity of valid paths for each subset S of $\{1, \dots, n\}$ is calculated.

Algorithm 2: $MinPath(G)$

Data: A graph $G = (V, E)$.

Result: Returns the numbering which leads to the $\phi_{\min}(G)$.

```

1  $DP[\rho(\{1, \dots, n\})] \leftarrow \infty$ 
2 for  $S \in \rho(\{1, \dots, n\})$  do
3   for  $v \in V$  do
4     if  $v \notin S$  then
5        $DP[S \cup \{v\}] \leftarrow \min(DP[S + \{v\}], DP[S] + VertexCost(v, S, G))$ 
6  $label[1 \dots n] \leftarrow 0$ 
7  $S \leftarrow \{1, 2, \dots, n\}$ 
8 while  $S \neq \emptyset$  do
9   for  $v \in V$  do
10    if  $v \in S$  then
11      if  $DP[S \setminus \{v\}] + VertexCost(v, S, G) = DP[S]$  then
12         $label[i] \leftarrow n - |S|$ 
13         $S \leftarrow S \setminus \{v\}$ 
14 return  $label$ 
```

The next part of the algorithm (Steps 6 to 13) uses the minimum quantity of valid paths found to determine an optimal numbering. In Step 6 a matrix $label$, with states for each number of

$\{1, \dots, n\}$, is created and initialised with 0's. In Step 7 the set $S = \{1, \dots, n\}$ is created. Steps 8 to 13 are iterated until S is empty. Steps 9 to 13 are iterated verifying every vertex $v \in V(G)$. In Step 10 is verified whether v still is in the set S . If true, in Step 11, it is checked if labelling v with $n - |S| + 1$ induces the minimum quantity of valid paths. If this is also true, the label of v is updated as $num - |S| + 1$, at Step 12, and v is removed from the set S at Step 13. In Step 14 the optimal *label* is returned.

The algorithm iterates through each subset of $\{1, \dots, n\}$, leading to a total of 2^n iterations. For each subset it iterates through every vertex of G and executes the *VertexCost* algorithm. The present algorithm runs through every vertex and every edge of G , leading to a complexity of $O(n^4 \cdot 2^n)$. It is important to point out that with some improvements, using masks of bits, the time complexity can be improved to $O(n \cdot 2^n)$. The algorithm which returns the numbering that leads to the value of function $\phi_{\max}(G)$ of some given graph G is similar to Algorithm 2 (*MinPath(G)*), with small changes in Steps 1 and 5.

5. Results on circulant graphs

This section describes results regarding the minimum number of valid paths in prefix circulant graphs and the maximum number of valid paths in suffix circulant graphs. Initially, the particular numbering used in both cases is presented. Furthermore, some definitions used in Theorems 5.6 and 5.9 are also presented. The minimum validity $\phi_{\min}(G)$ of prefix circulant graphs and the maximum validity $\phi_{\max}(G)$ of suffix circulant graphs are shown to be represented as closed formulas in Theorems 5.9 and 5.10, respectively.

Definition 5.1 *The particular numbering π^I , of any graph $G = (V(G), E(G))$ of order n , that is defined as*

$$\pi^I(v_i) = i, v_i \in V(G), i = 1, \dots, n, \quad (7)$$

is termed the identity numbering.

Definition 5.2 *Given a graph $G = (V(G), E(G))$, a vertex $u \in V(G)$ and a numbering π , the number of valid paths induced by u in π is equal to $\binom{q_u}{2}$, with q_u being the quantity of vertices v such that $\pi(u) < \pi(v)$ and $(u, v) \in E(G)$.*

Definition 5.3 *If $G = (V(G), E(G)) = C_n(R)$ is a circulant graph with distinct vertices $u, v \in V(G)$, we define the following parameters of G :*

$$EQ(u, v) = |\{x \in V(G) \mid \pi^I(u) < \pi^I(v) < \pi^I(x) \text{ and } \{(u, x), (v, x)\} \in E(G)\}|; \quad (8)$$

$$NEQ(u, v) = |\{x \in V(G) \mid \pi^I(u) < \pi^I(x) < \pi^I(v) \text{ and } \{(u, x), (v, x)\} \in E(G)\}|; \quad (9)$$

$$T(u, v) = |\{x \in V(G) \mid \pi^I(u) < \pi^I(x) < \pi^I(v), (u, x) \in E(G), (v, x) \notin E(G)\}|; \quad (10)$$

$$P(u, v) = |\{x \in V(G) \mid \pi^I(u) < \pi^I(v) < \pi^I(x), (u, x) \in E(G), (v, x) \notin E(G)\}|; \quad (11)$$

$$Pr(u, v) = |\{x \in V(G) \mid \pi^I(u) < \pi^I(v) < \pi^I(x), (u, x) \notin E(G), (v, x) \in E(G)\}|; \quad (12)$$

$$D(u, v) = \pi^I(v) - \pi^I(u). \quad (13)$$

$EQ(u, v)$, $NEQ(u, v)$, $T(u, v)$, $P(u, v)$ and $Pr(u, v)$ are the cardinalities of particular subsets of vertices of $V(G)$ and are used in further proofs. $EQ(u, v)$ represents the quantity of vertices that are adjacent to both u and v and is labelled with a number that is greater than both $\pi^I(u)$ and $\pi^I(v)$. The other cardinalities can be calculated similarly, with a different order of their labels or a different adjacency relationship.

Lemma 5.4 Given a circulant graph $G = C_n(R) = (V(G), E(G))$ and vertices $u, v \in V(G)$, then $T(u, v)$ is equal to the quantity of vertices x such that $\pi^I(u) < \pi^I(x) < \pi^I(v)$, $(u, x) \notin E(G)$ and $(v, x) \in E(G)$.

The proof of Lemma 5.4 is based on the construction of circulant graphs. Since it is simple, but long, it is omitted.

Lemma 5.5 Let $G = C_n(R) = (V(G), E(G))$ be a circulant graph and π^I be a numbering of G . If the labels $\pi^I(u)$ and $\pi^I(v)$ of distinct vertices $u, v \in V(G)$, where $\pi^I(u) < \pi^I(v)$, are swapped, then a new numbering δ say, is created. A vertex $x \in V(G)$, distinct from u and v , possibly induces in δ a different number of valid paths if $\pi^I(u) < \pi^I(x) < \pi^I(v)$.

Proof.

If edge $(u, x) \in E(G)$, since $\pi^I(u) < \pi^I(x)$, x cannot induce a valid path in π^I that begins with edge (u, x) . However, when $\pi^I(u)$ and $\pi^I(v)$ are swapped, since $\pi^I(x) < \pi^I(v)$, x may possibly induce a valid path in π^I that begins with edge (u, x) . In this case, x will induce in δ a new valid path $\langle u, x, w \rangle$, for some vertex $w \in V(G)$, distinct from u , x and v , only if edge $(x, w) \in E(G)$ and $\pi^I(x) < \pi^I(w)$. □

Theorem 5.6 If $PC_n(R)$ is a prefix circulant graph and π^I is the identity numbering given by Definition 5.1, then

$$\phi_{\pi^I}(PC_n(R)) = \sum_{i=|R|+1}^{2 \cdot |R|} \binom{i}{2} + (n - 2 \cdot |R|) \cdot \binom{|R|}{2} + \sum_{i=0}^{|R|-1} \binom{i}{2}.$$

Proof. Let the graph $PC_n(R)$ be denoted by just G . The following cases cover all possible $v_i \in V(G)$.

Case 1 The vertices v_i , such that $1 \leq i \leq |R|$, in the graph G induce in π^I the total of $\sum_{i=|R|+1}^{2 \cdot |R|} \binom{i}{2}$ valid paths. The vertex v_1 is labelled as $\pi^I(v_1) = 1$, the vertex v_2 is labelled as $\pi^I(v_2) = 2$ and the last vertex $v_{|R|}$ is labelled as $\pi^I(v_{|R|}) = |R|$. They are all adjacent to each other, so $v_{|R|}$ is adjacent to $|R| - 1$ vertices y such that $\pi^I(y) < \pi^I(v_{|R|})$, the vertex before $v_{|R|}$ is adjacent to $|R| - 2$ vertices and so on, until the vertex v_1 which is adjacent only to vertices with labels greater than its own label. This induces a quantity of valid paths equal to the sum in the statement of the present theorem.

Case 2 The vertices v_i , such that $|R| < i \leq n - |R|$, in the graph G will each induce in π^I the total of $\binom{|R|}{2}$ valid paths. The set of edges in each v_i will have the form:

$$\{v_{i-|R|}, v_{i-|R|+1}, \dots, v_{i-1}, v_{i+1}, \dots, v_{i+|R|-1}, v_{i+|R|}\}.$$

Thus, the set of labels of the vertices are:

$$\{\pi^I(v_{i-|R|}), \pi^I(v_{i-|R|+1}), \dots, \pi^I(v_{i-1}), \pi^I(v_{i+1}), \dots, \pi^I(v_{i+|R|-1}), \pi^I(v_{i+|R|})\}$$

and

$$\{i - |R|, i - |R| + 1, \dots, i - 1, i + 1, \dots, i + |R| - 1, i + |R|\}.$$

Therefore, each of them is adjacent to $|R|$ vertices y which will have $\pi^I(y) > \pi^I(x)$, inducing a quantity of valid paths equal to the sum in the statement of the present theorem.

Case 3 The vertices v_i , such that $n - |R| < i \leq n$, in the graph G induce in π^I the total of $\sum_{i=0}^{|R|-1} \binom{i}{2}$ valid paths. The vertex v_n is labelled as $\pi^I(v_n) = n$, the next vertex v_{n-1} is labelled as $\pi^I(v_{n-1}) = n - 1$ and the vertex $v_{n-(|R|-1)}$ is labelled as $\pi^I(v_{n-(|R|-1)}) = n - |R| + 1$. They are all adjacent to each other, so $v_{n-(|R|-1)}$ is adjacent to $|R| - 1$ vertices y such that $\pi^I(y) > \pi^I(v_{n-(|R|-1)})$. The vertex before $v_{n-(|R|-1)}$ is adjacent to $|R| - 2$ vertices and so on, until the vertex v_n which is adjacent only to vertices with labels lower than its own. This induces the quantity of valid paths equal to the sum in the statement of the present theorem. □

Definition 5.7 Let $G = PC_n(R) = (V, E)$ be a prefix circulant graph:

- (i) $B = \{v_i \mid (v_i) \in V, i \leq |R|\}$ contains the first $|R|_{th}$ vertices of $PC_n(R)$, which induce in π^I a total of $\sum_{i=|R|+1}^{2|R|} \binom{i}{2}$ valid paths;
- (ii) $C = \{v_i \mid (v_i) \in V, |R| < i \leq n - |R|\}$ contains the next $(n - 2|R|)_{th}$ vertices, which induce in π^I a total of $(n - 2|R|) \cdot \binom{|R|}{2}$ valid paths.
- (iii) $S = \{v_i \mid (v_i) \in V(G), n - |R| < i \leq n\}$ contains the last $|R|_{th}$ vertices, which induce in π^I a total of $\sum_{i=0}^{|R|-1} \binom{i}{2}$ valid paths.

Lemma 5.8 If $PC_n(R)$ is a prefix circulant graph, π^I is the numbering given by Definition 5.1, and u, v is any pair of distinct vertices in $PC_n(R)$ such that $\pi^I(u) < \pi^I(v)$, then the quantity of valid paths induced by u and v in π^I is less than or equal to the quantity of valid paths induced by u and v in a numbering δ , where:

$$\delta(x) = \begin{cases} \pi^I(u), & \text{if } x = v; \\ \pi^I(v), & \text{if } x = u; \\ \pi^I(x), & \text{otherwise.} \end{cases} \quad \forall x \in PC_n(R). \quad (14)$$

Proof. The quantity of valid paths induced by u and v in π^I can be written as $\binom{q_u}{2} + \binom{q_v}{2}$ such that $q_u = NEQ(u, v) + EQ(u, v) + T(u, v) + P(u, v)$ and $q_v = EQ(u, v) + Pr(u, v)$.

When the u and v labels are swapped, the new valid paths induced by both will be $\binom{q'_u}{2} + \binom{q'_v}{2}$ where:

$$\begin{aligned} q'_u &= NEQ(u, v) + EQ(u, v) + T(u, v) + Pr(u, v), \\ q'_v &= EQ(u, v) + P(u, v) \end{aligned}$$

By hypothesis:

$$\left(\frac{NEQ(u, v) + EQ(u, v) + T(u, v) + P(u, v)}{2} \right) + \left(\frac{EQ(u, v) + Pr(u, v)}{2} \right) \leq \left(\frac{NEQ(u, v) + EQ(u, v) + T(u, v) + Pr(u, v)}{2} \right) + \left(\frac{EQ(u, v) + P(u, v)}{2} \right).$$

Some basic algebraic manipulation leads to:

$$\frac{2 \cdot (NEQ(u, v) + T(u, v))}{2} \cdot P(u, v) \leq \frac{2 \cdot (NEQ(u, v) + T(u, v))}{2} \cdot Pr(u, v)$$

and

$$P(u, v) \leq Pr(u, v);$$

which always is true for prefix circulant graphs since their connection set is inversely proportional to the numbering π^I . □

Theorem 5.9 If $PC_n(R)$ is a prefix circulant graph and π^I is the numbering given by Definition 5.1, then

$$\phi_{\pi^I}(PC_n(R)) = \phi_{\min}(PC_n(R)). \quad (15)$$

Proof. Let $PC_n(R)$ be denoted by the graph G . Suppose that $\phi_{\pi^I}(G) \neq \phi_{\min}(G)$, then there must exist some numbering δ such that $\phi_{\pi^I}(G) > \phi_{\delta}(G)$. Therefore, there is at least one label swapping operation of some pair of vertices $u, v \in V(G)$ that increases the quantity of valid paths. The results of the quantity of valid paths induced by u and by v are already proven by Lemma 5.8, so we are only going to analyse the valid paths induced by the other vertices. The cases below cover all possible swaps between any pair of vertices belonging to the sets B , C and S listed in Definition 5.7. All the cases rely on the following statement:

Remark 1 By Lemma 5.5 a new valid path must be induced by a vertex x such that $\pi^I(u) < \pi^I(x) < \pi^I(v)$.

Case 1 ($u, v \in B$): By Remark 1, it follows that $x \in B$. We now analyse the induced subgraph H of G such that $x \in V(H)$ if $x \in V(G)$ and $\pi^I(u) < \pi^I(x) < \pi^I(v)$. Since B is complete, if $x \in H$ then $(x, u), (x, v) \in E(H)$. Therefore, the quantity of valid paths induced by x in a new numbering δ , constructed by the label swap operation, does not change the quantity given by the numbering π .

Case 2 ($u, v \in S$): By Remark 1, it follows that $x \in S$. We now analyse the induced subgraph H of G such that $x \in V(H)$ if $x \in V(G)$ and $\pi^I(u) < \pi^I(x) < \pi^I(v)$. Since there is an edge between any pair of vertices in S , if $x \in H$ then $(x, u), (x, v) \in E(H)$. Therefore, the quantity of valid paths induced by x in a new numbering δ , constructed by the label swap operation, does not change the such quantity given by the numbering π .

Case 3 ($u, v \in C$): By Remark 1, it follows that $x \in C$. We now analyse the induced subgraph H of G such that $x \in V(H)$ if $x \in V(G)$ and $\pi^I(u) < \pi^I(x) < \pi^I(v)$.

$(x, u), (x, v) \in E(H) \implies$ the quantity of valid paths induced by x in δ remains the same.

$(x, u), (x, v) \notin E(H) \implies$ the quantity of valid paths induced by x in δ remains the same.

$(x, u) \in E(H)$ and $(x, v) \notin E(H) \implies$ by Definition 5.2, the quantity of valid paths induced by x in π^I is $\binom{q_x}{2}$, for some q_x . Note that q_x will be increased by 1 because $\pi^I(u) < \pi^I(x) < \pi^I(v)$.

$(x, u) \notin E(H)$ and $(x, v) \in E(H) \implies$ by Definition 5.2, the quantity of valid paths induced by x in π^I is $\binom{q_x}{2}$. Thus q_x will decrease by 1 because $\pi^I(u) < \pi^I(x) < \pi^I(v)$.

By Definition 5.7 (ii), the total quantity of valid paths induced by the vertices between u and v is a sub-segment of $\sum_{i=1}^{n-2|R|} \binom{|R|}{2}$, that is $\sum_{x_i \in V(H)} \binom{q_{x_i}}{2}$. Thus, the sum τ of the quantities of valid paths induced by all the vertices in H is:

$$\tau = \binom{q_u}{2} + \binom{q_v}{2} + \sum_{\substack{(x_i, u) \notin E(H), \\ (x_i, v) \in E(H)}} \binom{q_{x_i}}{2} + \sum_{\substack{(x_i, u), (x_i, v) \notin E(H) \vee \\ (x_i, u), (x_i, v) \in E(H)}} \binom{q_{x_i}}{2} + \sum_{\substack{(x_i, u) \in E(H), \\ (x_i, v) \notin E(H)}} \binom{q_{x_i}}{2}.$$

The only part that will change in the new permutation δ is:

$$\sum_{\substack{(x_i, u) \notin E(H), \\ (x_i, v) \in E(H)}} \binom{q_{x_i}}{2} + \sum_{\substack{(x_i, u) \in E(H), \\ (x_i, v) \notin E(H)}} \binom{q_{x_i}}{2},$$

which can be replaced by the sum:

$$\sum_{\substack{(x_i, u) \notin E(H), \\ (x_i, v) \in E(H)}} \binom{q_{x_i} - 1}{2} + \sum_{\substack{(x_i, u) \in E(H), \\ (x_i, v) \notin E(H)}} \binom{q_{x_i} + 1}{2}.$$

By Lemma 5.4 the total quantity of vertices $x_1 \in C$ such that both $(x_1, u) \in E(H)$ and $(x_1, v) \notin E(H)$, is the same as the total quantity of vertices $x_2 \in C$ such that $(x_2, v) \in E(H)$ and $(x_2, u) \notin E(H)$, and is equal to $T(u, v)$. Then the previous sums can be rewritten as:

$$\tau_\pi = \sum_{i=1}^{T(u, v)} \binom{|R|}{2} + \sum_{i=1}^{T(u, v)} \binom{|R|}{2},$$

that can be expressed as:

$$\tau_\delta = \sum_{i=1}^{T(u, v)} \binom{|R| - 1}{2} + \sum_{i=1}^{T(u, v)} \binom{|R| + 1}{2}.$$

Thus,

$$\begin{aligned} \tau_\pi - \tau_\delta &= 2 \cdot \sum_{i=1}^{T(u, v)} \frac{(|R|)(|R| - 1)}{2} - \left(\sum_{i=1}^{T(u, v)} \frac{(|R| - 1)(|R| - 2)}{2} + \sum_{i=1}^{T(u, v)} \frac{(|R| + 1)(|R|)}{2} \right), \\ &= T(u, v) \cdot (|R|^2 - |R|) - T(u, v) \cdot (|R|^2 - |R| + 1), \\ &= -T(u, v). \end{aligned}$$

Therefore,

$$\tau_\pi = \tau_\delta - T(u, v).$$

The proofs of **Case 4** ($u \in B, v \in C$), **Case 5** ($u \in C, v \in S$) and **Case 6** ($u \in B, v \in S$) are similar to the proof of **Case 3** and are omitted.

Therefore, by contradiction, $\phi_{\pi^I}(G) = \phi_{\min}(G)$. □

Theorem 5.10, given next, is analogous to Theorems 5.6 and 5.9, but related to suffix circulant graphs. Its proof is omitted since it is similar to the proofs of the latter two theorems.

Theorem 5.10 *If $SC_n(R)$ is a suffix circulant graph and π^I is the identity numbering given by Definition 5.1, then*

$$\phi_{\pi^I}(SC_n(R)) = \sum_{i=0}^{2|R|-1} \binom{i}{2} + \left(\frac{n}{2} - |R| \right) \cdot \binom{2|R|-1}{2} = \binom{2|R|}{3} + \left(\frac{n}{2} - |R| \right) \cdot \binom{2|R|-1}{2}. \quad (16)$$

and

$$\phi_{\pi^I}(SC_n(R)) = \phi_{\min}(SC_n(R)). \quad (17)$$

6. Conclusion

The *Valid Path problem* involves finding a numbering that optimises the number of valid paths in a given graph (cf Section 3). The focus of this work is the specific class of circulant graphs (cf Section 2). Two sub-classes, denoted as prefix circulant graphs and suffix circulant graphs, were defined and their behaviour regarding the Valid Path Problem was established (cf Section 5).

The minimum validity $\phi_{\min}(G)$ of prefix circulant graphs was proved as the closed formula (5.9). The maximum validity $\phi_{\max}(G)$ of suffix circulant graphs has also been proved as the

closed formula (5.10). Is important to state that these classes generalise some well known classes of graphs, such as cycles, complete graphs and powers of cycles.

Another important result achieved in this work is the development of algorithms (cf Section 4) that determine numberings that induce $\phi_{\min}(G)$ and $\phi_{\max}(G)$ valid paths in an arbitrary graph G . Although the proposed algorithm does not have polynomial time complexity, it is significantly faster than the brute force approach, that has $O(n!)$ complexity.

6.1. Future Work

Since the results obtained here do not cover all the graphs in the circulant graph class, we plan to complete the study of the behaviour of the *Path Validity Problem* in the remaining graphs in the class. Foulds and Longo [2023] proposed the Conjectures 6.1 and 6.2, given below, the settling of which are currently among our research objectives:

Conjecture 6.1 *MIN-VP is an $\mathcal{NP}$ -complete problem.*

Conjecture 6.2 *MAX-VP is an $\mathcal{NP}$ -complete problem.*

Some of the results on particular classes of graphs obtained by Foulds and Longo [2023] are still incomplete. Reviewing and finalising these results is also our intention.

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