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Some algebraic properties of Sierpiński-type graphs*

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Abstract

This paper deals with some algebraic properties of Sierpiński graphs and a family of regular generalized Sierpiński graphs. For the family of regular generalized Sierpiński graphs, we obtain their spectrum and characterize those graphs that are Cayley graphs. As a by-product, a new family of non-Cayley vertex-transitive graphs, and consequently, a new set of non-Cayley numbers are introduced. We also obtain the Laplacian spectrum of Sierpiński graphs in some particular cases, and make a conjecture on the general case.

Keywords: Sierpiński graph, spectrum, Laplacian, Cayley graph, non-Cayley number.

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1 Introduction

Sierpiński-type graphs show up in a wide range of areas; for instance, physics, dynamical systems, probability, and topology, to name a few. The Sierpiński gasket graphs form one of the most significant families of such graphs that are obtained by a finite number of iterations that give the Sierpiński gasket in the limit. Several more families of Sierpiński-type graphs have been introduced and studied in the literature (see Barrière, Comellas, and Dalfó [1] and Hinz, Klavžar, and Zemljič [6]). In this paper, we deal with two families of them, as described below.

For positive integers n, k , the *Sierpiński graph* $S(n, k)$ is defined with vertex set $[k]^n$, where $[k] := \{1, \dots, k\}$, and two different vertices (u_1, \dots, u_n) and (v_1, \dots, v_n) are adjacent if and only if there exists a $t \in [n]$ such that

- $u_i = v_i$ for $i = 1, \dots, t - 1$,
- $u_t \neq v_t$,
- $u_j = v_t$ and $v_j = u_t$ for $j = t + 1, \dots, n$.

For instance, the graphs $S(3, 3)$ and $S(2, 4)$ are depicted in Figure 1.

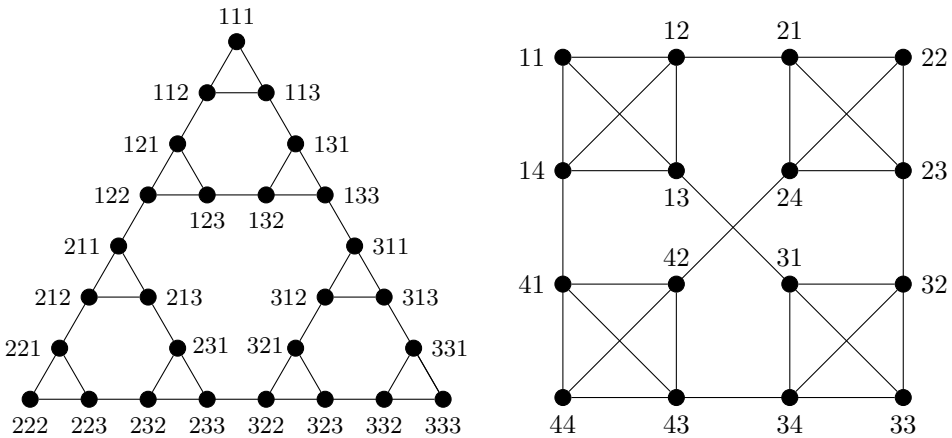


Figure 1: The Sierpiński graphs $S(3, 3)$ (left) and $S(2, 4)$ (right).

Sierpiński graphs $S(n, k)$ were introduced in Klavžar and Milutinović [8]. The graph $S(n, 3)$ is indeed isomorphic to the graph of the Tower of Hanoi with n disks. The graph $S(n, k)$ has $k^n - k$ vertices of degree k and k vertices of degree $k - 1$ that are (i, \dots, i) for $i \in [k]$. These vertices are called the *extreme vertices*.

In addition to $S(n, k)$, we consider a ‘regularization’ of them as another family of Sierpiński-type graphs. The graphs $S^{++}(n, k)$, introduced in Klavžar and Mohar [9], are defined as follows. The graph $S^{++}(1, k)$ is the complete graph K_{k+1} . For $n \geq 2$, $S^{++}(n, k)$ is the graph obtained from the disjoint union of $k + 1$ copies of $S(n - 1, k)$ in which the extreme vertices in distinct copies of $S(n - 1, k)$ are connected as the complete graph K_{k+1} . See Figure 2 for an illustration of $S^{++}(3, 3)$.

Many properties of Sierpiński-type graphs, including those of $S(n, k)$ and $S^{++}(n, k)$, have been studied in the literature, for a survey see Hinz, Klavžar, and Zemljič [6]. In

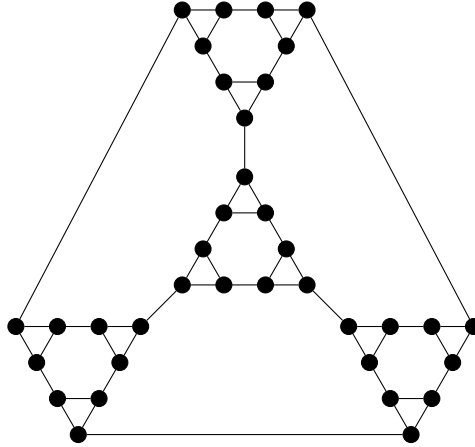


Figure 2: The graph $S^{++}(3, 3)$.

this paper, we investigate some algebraic properties of the two families of graphs, namely the spectrum and the property of being a Cayley graph. More precisely, in Section 2, we determine the spectrum of the graphs $S^{++}(n, k)$. The Laplacian spectrum of $S(n, k)$ is already known for $k = 2, 3$. We establish the case $n = 2$, in Section 3, and make a conjecture on the Laplacian spectrum of $S(n, k)$ in general. We also characterize the graphs $S^{++}(n, k)$ that are Cayley graphs in Section 4. As a by-product, a new family of non-Cayley vertex-transitive graphs are obtained. From this result, we conclude a new set of square-free non-Cayley numbers in Section 5, and we discuss its distribution.

2 Spectrum of $S^{++}(n, k)$

Let Γ be a simple graph with vertex set $V(\Gamma) = \{v_1, \dots, v_n\}$ and edge set $E(\Gamma)$. Its adjacency matrix $A(\Gamma) = [a_{ij}]$ is an $n \times n$ symmetric matrix with $a_{ij} = 1$ if v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. The multi-set of the eigenvalues of $A(\Gamma)$ is called the spectrum of Γ .

In this section, we determine the spectrum of $S^{++}(n, k)$. As we will see, the recursive structure of these Sierpiński-type graphs also shows up in their spectrum. We first recall some basic facts.

The incidence matrix of a graph Γ is a 0-1 matrix $X(\Gamma) = [x_{ve}]$, with rows indexed by the vertices and columns indexed by the edges of Γ , where $x_{ve} = 1$ if the vertex v is an endpoint of the edge e . For a graph Γ , $\mathcal{L}(\Gamma)$ denotes the line graph of Γ , in which $V(\mathcal{L}(\Gamma))$ corresponds with $E(\Gamma)$, and two vertices of $\mathcal{L}(\Gamma)$ are adjacent if and only if they have a common vertex as edges of Γ . The subdivision graph $\mathcal{S}(\Gamma)$ of Γ is the graph obtained by inserting a new vertex into every edge of Γ . It is easy to verify that

$$X(\Gamma)^\top X(\Gamma) = 2I + A(\mathcal{L}(\Gamma)), \tag{2.1}$$

and, moreover, if Γ is k -regular, then

$$X(\Gamma)X(\Gamma)^\top = kI + A(\Gamma). \tag{2.2}$$

The following lemma gives a recursive relation for the graphs $S^{++}(n, k)$.

Lemma 2.1. *The graph $S^{++}(n + 1, k)$ is isomorphic to $\mathcal{L}(\mathcal{S}(S^{++}(n, k)))$.*

Proof. Let k be fixed. The graph $\Gamma_n := S^{++}(n, k)$ can be obtained by the union of $S(n, k)$ and $S(n - 1, k)$ by adding a matching between the extreme vertices of the two graphs. If we consider $\{0\} \times [k]^{n-1}$ as the vertex set of $S(n - 1, k)$ (to make them compatible with the length n of the vertices of $S(n, k)$), then $(\{0\} \cup [k]) \times [k]^{n-1}$ is the vertex set of Γ_n . It follows that any edge $e = \{\mathbf{u}, \mathbf{v}\}$ of Γ_n is of one of the following types:

- (1) $\mathbf{u} = (u_1, \dots, u_r, u, v, \dots, v)$, $\mathbf{v} = (u_1, \dots, u_r, v, u, \dots, u)$ for some $r \leq n - 2$ and $u \neq v$;
- (2) $\mathbf{u} = (u_1, \dots, u_{n-1}, u)$, $\mathbf{v} = (u_1, \dots, u_{n-1}, v)$ with $u \neq v$;
- (3) $\mathbf{u} = (0, u, \dots, u)$, $\mathbf{v} = (u, u, \dots, u)$.

Each $e = \{\mathbf{u}, \mathbf{v}\} \in E(\Gamma_n)$ is divided into two new edges $e_{\mathbf{u}}$ and $e_{\mathbf{v}}$ in $\mathcal{S}(\Gamma_n)$, where we assume that $\mathbf{u} \in e_{\mathbf{u}}$ and $\mathbf{v} \in e_{\mathbf{v}}$. We define a map $\psi: E(\mathcal{S}(\Gamma_n)) \rightarrow (\{0\} \cup [k]) \times [k]^n$ based on the type of e as follows:

- (i) If e is of type (1) or (2), then $\psi(e_{\mathbf{u}}) = (\mathbf{u}, v)$ and $\psi(e_{\mathbf{v}}) = (\mathbf{v}, u)$;
- (ii) If e is of type (3), then $\psi(e_{\mathbf{u}}) = (\mathbf{u}, u)$ and $\psi(e_{\mathbf{v}}) = (\mathbf{v}, u)$.

It is easily seen that ψ is a one-to-one map. We show that ψ is an isomorphism from $\mathcal{L}(\mathcal{S}(\Gamma_n))$ to Γ_{n+1} . Let e and e' be two edges that share a vertex \mathbf{x} of $\mathcal{S}(\Gamma_n)$. If $\mathbf{x} = (x_1, \dots, x_n)$ is an ‘old’ vertex of $\mathcal{S}(\Gamma_n)$, then $\psi(e) = (\mathbf{x}, y)$ and $\psi(e') = (\mathbf{x}, z)$ for some $y \neq z$. Then, it is clear that $\psi(e)$ and $\psi(e')$ are adjacent in Γ_{n+1} . If \mathbf{x} is a ‘new’ vertex of $\mathcal{S}(\Gamma_n)$, then from (i) and (ii), it is clear that $\psi(e)$ and $\psi(e')$ are adjacent in Γ_{n+1} . This shows that ψ is indeed a one-to-one homomorphism. As $\mathcal{L}(\mathcal{S}(\Gamma_n))$ and Γ_{n+1} have the same number of edges, it follows that ψ is an isomorphism. \square

We recall that if A is a non-singular square matrix, then

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = |A| \cdot |D - CA^{-1}B|, \tag{2.3}$$

where $|\cdot|$ denotes the determinant of a matrix. Also, recall that if M is a $p \times q$ matrix, then

$$|xI - MM^T| = x^{p-q}|xI - M^T M|. \tag{2.4}$$

(Note that (2.4) might not be valid if $p \leq q$ and $x = 0$, but this has no effect in our argument since two polynomials that agree in all but finitely many points, agree everywhere.)

Let

$$f(x) = x^2 + (2 - k)x - k, \tag{2.5}$$

and let $f^j(x)$ denote the polynomial of degree 2^j obtained by j times composition of f with itself. As a convention, we let $f^0(x) = x$.

We now give the main result of this section.

Theorem 2.2. *Let k be an integer and $P_n(x)$ denote the characteristic polynomial of the adjacency matrix of $S^{++}(n, k)$. Then, P_n satisfies the recursion relation*

$$P_n(x) = (x(x + 2))^{k^{n-2} \binom{k}{2} - 1} P_{n-1}(f(x)), \quad n \geq 2, \tag{2.6}$$

with $P_1(x) = (x - k)(x + 1)^k$. Moreover, for $n \geq 2$, the spectrum of $S^{++}(n, k)$ consists of the following eigenvalues:

- (i) k with multiplicity 1,
- (ii) the zeros of $f^{n-1}(x) + 1$ each with multiplicity k ,
- (iii) the zeros of $f^j(x)$ each with multiplicity $k^{n-2-j} \left(\binom{k}{2} - 1 \right)$ for $j = 0, 1, \dots, n - 2$,
- (iv) the zeros of $f^j(x) + 2$ each with multiplicity $k^{n-2-j} \left(\binom{k}{2} - 1 \right) + 1$ for $j = 0, 1, \dots, n - 2$.

Proof. Let $\Gamma_n := S^{++}(n, k)$. Suppose that X and Y are the incidence matrices of Γ_{n-1} and $\mathcal{S}(\Gamma_{n-1})$, respectively. By Lemma 2.1, Γ_n is isomorphic to $\mathcal{L}(\mathcal{S}(\Gamma_{n-1}))$. It follows that

$$YY^\top = \begin{bmatrix} kI_p & X \\ X^\top & 2I_q \end{bmatrix},$$

where the matrix is divided according to the partition of the vertices into $p = k^{n-1} + k^{n-2}$ ‘old’ vertices of Γ_{n-1} and $q = \frac{1}{2}(k^n + k^{n-1})$ ‘new’ vertices (which have degree 2) added to Γ_{n-1} to obtain $\mathcal{S}(\Gamma_{n-1})$. Therefore, from (2.3),

$$\begin{aligned} |xI - YY^\top| &= |(x - k)I_p| \cdot \left| (x - 2)I_q - X^\top ((x - k)I_p)^{-1} X \right| \\ &= (x - k)^p \left| (x - 2)I_q - \frac{1}{x - k} X^\top X \right| \\ &= (x - k)^{p-q} \left| (x - 2)(x - k)I_q - X^\top X \right| \\ &= (x - k)^{p-q} \left| (x - 2)(x - k)^{q-p} \left| (x - 2)(x - k)I_p - XX^\top \right| \right| \quad \text{(by (2.4))} \\ &= (x - 2)^{q-p} \left| ((x - 2)(x - k) - k)I_p - A(\Gamma_{n-1}) \right| \quad \text{(by (2.2))} \\ &= (x - 2)^{q-p} P_{n-1}((x - 2)(x - k) - k). \end{aligned} \tag{2.7}$$

On the other hand, by (2.1) and (2.2), we have

$$P_n(x) = |(x + 2)I_{2q} - Y^\top Y| = (x + 2)^{q-p} |(x + 2)I_{p+q} - YY^\top|.$$

Now, from (2.7) it follows that

$$P_n(x) = (x(x + 2))^{q-p} P_{n-1}(x(x + 2 - k) - k),$$

implying (2.6).

To prove the second part of the theorem, note that as $\Gamma_1 = K_{k+1}$, we have $P_1(x) = (x - k)(x + 1)^k$. From (2.6), we conclude that

$$P_2(x) = (x(x + 2))^{\binom{k}{2} - 1} (f(x) - k)(f(x) + 1)^k,$$

and since

$$f(x) - k = (x + 2)(x - k), \tag{2.8}$$

the assertion follows for $n = 2$. Now assume that $n \geq 3$ and the assertion holds for $n - 1$. So, we have

$$P_{n-1}(x) = (x - k) (f^{n-2}(x) + 1)^k \prod_{j=0}^{n-3} (f^j(x))^{m_{n-3-j}} (f^j(x) + 2)^{1+m_{n-3-j}},$$

in which $m_i = k^i \left(\binom{k}{2} - 1 \right)$. It follows that

$$P_{n-1}(f(x)) = (f(x) - k) (f^{n-1}(x) + 1)^k \prod_{j=1}^{n-2} (f^j(x))^{m_{n-2-j}} (f^j(x) + 2)^{1+m_{n-2-j}}.$$

This, together with (2.6) and (2.8), implies the result. □

Remark 2.3. It is straightforward to see that the zeros of $f^j(x)$ and $f^j(x) + 2$ for $j = 1$ are $\frac{1}{2}(k - 2 \pm \sqrt{k^2 + 4})$ and $\frac{1}{2}(k - 2 \pm \sqrt{k^2 - 4})$, respectively, and for $j \geq 2$ are of the form

$$\frac{1}{2}(k - 2) \pm \frac{1}{2} \sqrt{k(k + 2) \pm 2 \sqrt{k(k + 2) \pm 2 \sqrt{\dots \pm 2 \sqrt{k^2 + 4}}}}$$

and

$$\frac{1}{2}(k - 2) \pm \frac{1}{2} \sqrt{k(k + 2) \pm 2 \sqrt{k(k + 2) \pm 2 \sqrt{\dots \pm 2 \sqrt{k^2 - 4}}}}$$

respectively, each of them consisting of j nested radicals in iterative forms. Moreover, the zeros of $f^{n-1}(x) + 1$ are

$$-1, k - 1, \frac{1}{2}(k - 2) \pm \frac{1}{2} \sqrt{k^2 + 4k}, \frac{1}{2}(k - 2) \pm \frac{1}{2} \sqrt{k(k + 2) \pm 2 \sqrt{k^2 + 4k}}, \dots, \\ \frac{1}{2}(k - 2) \pm \frac{1}{2} \sqrt{k(k + 2) \pm 2 \sqrt{k(k + 2) \pm 2 \sqrt{\dots \pm 2 \sqrt{k^2 + 4k}}}}$$

where the last one consists of $n - 2$ nested radicals.

3 Laplacian spectrum of $S(n, k)$

For a graph Γ , the matrix $L(\Gamma) = D(\Gamma) - A(\Gamma)$ is the *Laplacian matrix* of Γ , where $D(\Gamma)$ is the diagonal matrix of vertex degrees. The multi-set of eigenvalues of $L(\Gamma)$ is called the *Laplacian spectrum* of Γ . In this section, we deal with the Laplacian spectrum of $S(n, k)$. This is trivial for $n = 1$ or $k = 1$. For $k = 2, 3$, the Laplacian spectrum of $S(n, k)$ is already known (see Remark 3.4 below). We establish the case $n = 2$, and put forward a conjecture explicitly describing the Laplacian spectrum of $S(n, k)$ in general.

Let E_{ij} be a $k \times k$ matrix in which all entries are 0, except the (i, j) entry that is 1. Consider the $k^2 \times k^2$ matrix

$$C := \sum_{i=1}^k \sum_{j=1}^k (E_{ij} \otimes E_{ji}),$$

where ‘ \otimes ’ denotes the Kronecker product. The matrix C is called the *commutation matrix*. The main property of the commutation matrix (see Magnus and Neudecker [10]) is that it commutes the Kronecker product: for any $k \times k$ matrices M, N ,

$$C(M \otimes N)C = N \otimes M.$$

Note that each row and each column of C corresponds with a pair (i, j) for $1 \leq i, j \leq k$. Moreover, C is indeed a permutation matrix in which the only 1 entry in the row (i, j) is located at the column (j, i) for every $1 \leq i, j \leq k$.

For $n = 1$, the Laplacian spectrum of $S(1, k) = K_k$ is $\{0^{[1]}, k^{[k-1]}\}$, where the superscripts indicate multiplicities. In the following theorem, we determine the Laplacian spectrum of $S(2, k)$.

Theorem 3.1. *The Laplacian spectrum of $S(2, k)$ is the following:*

$$\left\{ 0^{[1]}, k^{\lfloor \binom{k}{2} \rfloor}, (k+2)^{\lfloor \binom{k-1}{2} \rfloor}, \left(\frac{1}{2}(k+2) \pm \frac{1}{2}\sqrt{k^2+4} \right)^{\lfloor \binom{k-1}{2} \rfloor} \right\}.$$

Proof. First, note that the graph $S(2, k)$ consists of k copies of K_k together with a matching M of size $\binom{k}{2}$; exactly one edge for each pair of copies of K_k . Let L denote the Laplacian matrix of $S(2, k)$, and L' be the Laplacian matrix of the induced subgraph by the edges of M . It is seen that $L = Q - B$, where $Q = L(kK_k) + I$ and $B = I - L'$. Note that B is a permutation matrix with $\binom{k}{2} + k$ eigenvalues 1 and $\binom{k}{2}$ eigenvalues -1 . Observe that Q has k eigenvalues 1 and $k^2 - k$ eigenvalues $k + 1$. We have the following bounds on the dimensions of intersections of the eigenspaces of B and Q :

$$\begin{aligned} \dim(\mathcal{E}_1(B) \cap \mathcal{E}_{k+1}(Q)) &\geq k^2 - k + \binom{k}{2} + k - k^2 = \binom{k}{2}, \\ \dim(\mathcal{E}_{-1}(B) \cap \mathcal{E}_{k+1}(Q)) &\geq k^2 - k + \binom{k}{2} - k^2 = \binom{k}{2} - k, \end{aligned}$$

in which \mathcal{E}_λ denotes the eigenspace corresponding to the eigenvalue λ . For $\mathbf{x} \in \mathcal{E}_1(B) \cap \mathcal{E}_{k+1}(Q)$, we have $L\mathbf{x} = k\mathbf{x}$ and for $\mathbf{x} \in \mathcal{E}_{-1}(B) \cap \mathcal{E}_{k+1}(Q)$, $L\mathbf{x} = (k+2)\mathbf{x}$. This means that L has eigenvalues k and $k+2$ with multiplicities at least $\binom{k}{2}$ and $\binom{k}{2} - k$, respectively.

We also have

$$Q = I_k \otimes ((k+1)I_k - J_k), \tag{3.1}$$

and from the eigenvalues of Q ,

$$Q^2 - (k+2)Q + (k+1)I = O. \tag{3.2}$$

Coming back to B , for each of the extreme vertices $(1, 1), \dots, (k, k)$ of $S(2, k)$, there is a 1 on all the entries of the diagonal of B . The off-diagonal 1’s correspond with the edges of M . By the definition of $S(2, k)$, the edges of M connect the vertices (i, j) and (j, i) for $i \neq j$. It turns out that B is the commutation matrix, and thus

$$BQB = ((k+1)I_k - J_k) \otimes I_k. \tag{3.3}$$

The right sides of (3.1) and (3.3) commute, and so

$$BQBQ = QBQB.$$

Next, we see that

$$\begin{aligned}
 &(L^2 - (k + 2)L + kI)(QB - BQ) \\
 &= ((Q - B)^2 - (k + 2)(Q - B) + kI)(QB - BQ) \\
 &= (Q^2 - (k + 2)Q + kI + B^2 + (k + 2)B - QB - BQ)(QB - BQ) \\
 &= ((k + 2)B - QB - BQ)(QB - BQ) \quad (\text{by (3.2) and since } B^2 = I) \\
 &= Q^2 - (k + 2)Q - B(Q^2 - (k + 2)Q)B - (QB)^2 + (BQ)^2 \\
 &= (BQ)^2 - (QB)^2 \\
 &= O.
 \end{aligned}$$

The above equality shows that every vector in the column space of $QB - BQ$ is an eigenvector for L with eigenvalue λ , where $\lambda^2 - (k + 2)\lambda + k = 0$. To obtain the multiplicity of such λ , we compute the rank of $QB - BQ$:

$$\begin{aligned}
 \text{rank}(QB - BQ) &= \text{rank}(Q - BQB) \\
 &= \text{rank}(I_k \otimes ((k + 1)I_k - J_k) - ((k + 1)I_k - J_k) \otimes I_k) \\
 &= \text{rank}(J_k \otimes I_k - I_k \otimes J_k) \\
 &= 2k - 2.
 \end{aligned} \tag{3.4}$$

To show (3.4), suppose P is a $k \times k$ matrix whose first column is $\frac{1}{\sqrt{k}}(1, \dots, 1)^T$ and that $PP^T = I_k$. Then, $J_k = P(kE_{11})P^T$, and so

$$J_k \otimes I_k - I_k \otimes J_k = (P \otimes P)((kE_{11} \otimes I_k) - (I_k \otimes kE_{11}))(P^T \otimes P^T).$$

Since $(kE_{11} \otimes I_k) - (I_k \otimes kE_{11})$ is a diagonal matrix having precisely $2k - 2$ non-zero entries in the columns $2, 3, \dots, k, k + 1, 2k + 1, 3k + 1, \dots, (k - 1)k + 1$, (3.4) follows.

As $x^2 - (k + 2)x + k$ is an irreducible polynomial, each of its roots is an eigenvalue of L with multiplicity at least $k - 1$. The matrix L has a 0 eigenvalue. Thus, we have obtained so far $\binom{k}{2} + \binom{k}{2} - k + 2(k - 1) + 1 = k^2 - 1$ eigenvalues of L . As the sum of the eigenvalues of L is twice the number of edges of $S(2, k)$, it follows that the remaining eigenvalue is $k + 2$. So the proof is complete. \square

Based on empirical evidence, we put forward the following conjecture.

Conjecture 3.2. For $n, k \geq 2$, the Laplacian spectrum of $S(n, k)$ consists of the following eigenvalues:

- (i) 0 with multiplicity 1.
- (ii) The zeros of $f^j(k - x)$, each with multiplicity $\frac{1}{2}(k^{n-j} - 2k^{n-j-1} + k)$ for $j = 0, 1, \dots, n - 1$, where f is given in (2.5).
- (iii) The zeros of $f^j(k - x) + 2$, each with multiplicity $\frac{1}{2}(k^{n-j-1} - 1)(k - 2)$ for $j = 0, 1, \dots, n - 2$.

Remark 3.3. The zeros of $f^j(k - x)$ and $f^j(k - x) + 2$ for $j = 1$ are $\frac{1}{2}(k + 2 \pm \sqrt{k^2 + 4})$ and $\frac{1}{2}(k + 2 \pm \sqrt{k^2 - 4})$, respectively, and for $j \geq 2$ are of the form

$$\frac{1}{2}(k + 2) \pm \frac{1}{2} \sqrt{k(k + 2) \pm 2 \sqrt{k(k + 2) \pm 2 \sqrt{\dots \pm 2 \sqrt{k^2 + 4}}}}$$

and

$$\frac{1}{2}(k + 2) \pm \frac{1}{2} \sqrt{k(k + 2) \pm 2 \sqrt{k(k + 2) \pm 2 \sqrt{\dots \pm 2 \sqrt{k^2 - 4}}}}$$

respectively, each of them consisting of j nested radicals.

Remark 3.4. The graph $S(n, 2)$ is the path graph on 2^n vertices. Proposition 3.5 below shows that Conjecture 3.2 holds for $S(n, 2)$. In Grigorchuk and Šunić [5], the spectrum of the Schreier graph Γ_n was determined. The graph Γ_n is, in fact, the graph obtained from $S(n, 3)$ by adding a loop on each extreme vertex. By the way the adjacency matrix of $A(\Gamma_n)$ is defined in [5], for each loop a 1 entry on the diagonal is considered, so that each row and column of $A(\Gamma_n)$ has constant sum 3. It is then observed that the Laplacian spectrum of $S(n, 3)$ can be deduced from the spectrum of Γ_n , which agrees with Conjecture 3.2. In summary, Conjecture 3.2 holds for $n = 2$ and for $k = 2, 3$.

It is known in the literature that the characteristic polynomial of the Laplacian matrix of a path can be expressed in terms of the Chebyshev polynomials. From this fact, for a path with 2^n vertices, we obtain the iterated form according to Conjecture 3.2. For the sake of completeness, we give its complete argument here.

Proposition 3.5. *The characteristic polynomial of the Laplacian matrix of the path graph on 2^n vertices is equal to $x \prod_{j=0}^{n-1} g^j(2 - x)$, where $g(x) = x^2 - 2$.*

Proof. Let ϕ_m be the characteristic polynomial of the Laplacian matrix of the path graph on m vertices. Let T_m and U_m be the Chebyshev polynomials of degree m of the first and the second kind, respectively. Then T_m is the only polynomial satisfying $T_m(\cos \theta) = \cos m\theta$ and $U_m(x) = \sin((m + 1) \arccos x) / \sin(\arccos x)$ (Snyder [18]). From the identities given in Cvetković, Doob, and Sachs [2, p. 220], it follows that $\phi_m(x) = xU_{m-1}(x/2 - 1)$. By successive use of the identity $U_{2k-1}(x) = 2T_k(x)U_{k-1}(x)$ (see [18, p. 98]), we get

$$U_{2^n-1}(x) = 2^{n-1}T_{2^{n-1}}(x)T_{2^{n-2}}(x) \cdots T_2(x)U_1(x).$$

Note that $U_1(x) = 2x$ and $T_2(x) = 2x^2 - 1$. It is seen that $2T_2(x/2 - 1) = x^2 - 4x + 2 = g(2 - x)$. This, together with the identity $T_{2k}(x) = T_2(T_k(x))$, implies that $2T_{2^j}(x/2 - 1) = g^j(2 - x)$. The proof is now complete. □

4 What $S^{++}(n, k)$ are Cayley graphs?

Recall that a graph Γ is *vertex-transitive* if for any two vertices u, v of Γ , there exists an automorphism σ of Γ such that $\sigma(u) = v$. Let G be a group and $C \subset G$ such that $1 \notin C$ and $c \in C$ implies that $c^{-1} \in C$. The *Cayley graph* $\text{Cay}(G, C)$ with the group G and the ‘connection set’ C is the graph with vertex set G in which vertex u is connected to v if and only if $vu^{-1} \in C$.

It is known that any Cayley graph is vertex-transitive. In the other way around, at least for small orders, it seems that the great majority of vertex-transitive graphs are Cayley graphs, see McKay and Praeger [12]. It is expected to continue to be this way for larger orders. In fact, it is conjectured in Praeger, Li, and Niemeyer [15] that most vertex-transitive graphs are Cayley graphs. In this section, we first determine what $S^{++}(n, k)$ are vertex-transitive and, then, classify $S^{++}(n, k)$ that are Cayley graphs.

Proposition 4.1. *The graph $S^{++}(n, k)$ is vertex-transitive if and only if either $n \leq 2$ or $k \leq 2$.*

Proof. We have $S^{++}(n, 1) \cong K_2$, $S^{++}(1, k) \cong K_{k+1}$, and $S^{++}(n, 2)$ is the cycle graph on $2^{n-1} \cdot 3$ vertices, which are all vertex-transitive graphs. By Lemma 2.1, $S^{++}(2, k)$ is isomorphic to $\mathcal{L}(\mathcal{S}(K_{k+1}))$. In the graph $\mathcal{S}(K_{k+1})$, the ‘new’ vertices are in one-to-one correspondence with 2-subsets of $[k + 1]$. It is then easy to see that that any permutation of $[k + 1]$ induces an automorphism of $\mathcal{S}(K_{k+1})$. Now, for a given pair of edges of $\mathcal{S}(K_{k+1})$ which can be represented as $e = \{i, \{i, j\}\}$ and $e' = \{j', \{i', j'\}\}$, the automorphism induced by a permutation σ that $\sigma(i) = i'$ and $\sigma(j) = j'$, maps e to e' . It follows that $\mathcal{S}(K_{k+1})$ is edge-transitive, and so $\mathcal{L}(\mathcal{S}(K_{k+1})) \cong S^{++}(2, k)$ is vertex-transitive. Hence, assume that $n \geq 3$ and $k \geq 3$. We observe that an extreme vertex of a copy Δ of $S(n - 1, k)$ in $\Gamma = S^{++}(n, k)$ cannot be mapped to a non-extreme vertex of Δ by any automorphism of Γ . To be more precise, let $\mathbf{u} = (1, \dots, 1, 1)$ and $\mathbf{v} = (1, \dots, 1, 2)$. It can be seen that \mathbf{u} is a cut vertex for the induced subgraph by the vertices at distance at most 3 from \mathbf{u} , while \mathbf{v} is not a cut vertex for the induced subgraph by the vertices at distance at most 3 from \mathbf{v} . It follows that \mathbf{u} cannot be mapped to \mathbf{v} by any automorphism of Γ , and thus Γ is not vertex-transitive. \square

From Proposition 4.1, it follows that the graphs $S^{++}(n, k)$ for $n \geq 3$ and $k \geq 3$ cannot be Cayley graphs. The graphs $S^{++}(n, 1)$, $S^{++}(n, 2)$, and $S^{++}(1, k)$ are all Cayley graphs. It remains to characterize what $S^{++}(2, k)$ are Cayley graphs for $k \geq 3$. This is our goal in the rest of this section.

Definition 4.2. Let Γ be a graph and Δ a subgraph of Γ . We say that Γ is *strongly Δ -partitioned* if:

- (i) The vertex set of Γ is partitioned by the vertex sets of copies $\Delta_0, \dots, \Delta_k$ of Δ .
- (ii) Apart from $\Delta_0, \dots, \Delta_k$, the graph Γ contains no further copies of Δ .

By the way $S^{++}(n, k)$ is defined, it is constructed based on $k + 1$ copies of $S(n - 1, k)$. The following proposition gives a structural property of $S^{++}(n, k)$ that it is indeed strongly $S(n - 1, k)$ -partitioned for $n \geq 2$ and $k \geq 3$. Note that this is not the case for $k = 2$ because $S^{++}(n, 2)$, that is a cycle with $3 \cdot 2^{n-1}$ vertices, contains more than three copies of $S(n - 1, 2)$, which is a path on 2^{n-1} vertices. Although we only need the case $n = 2$ of the proposition, we state it in its full generality because it could be of independent interest.

Proposition 4.3. *Let $n \geq 2$ and $k \geq 3$. The graph $S^{++}(n, k)$ is strongly $S(n - 1, k)$ -partitioned.*

Proof. Let $\Gamma := S^{++}(n, k)$ and $\Gamma_0, \dots, \Gamma_k$ be the $k + 1$ copies of $S(n - 1, k)$ used to construct Γ by its definition. Clearly, $V(\Gamma_0), \dots, V(\Gamma_k)$ is a partition of $V(\Gamma)$. We show that Γ contains no more copies of $S(n - 1, k)$. Let Δ be a subgraph of Γ isomorphic to $S(n - 1, k)$.

First, assume that $n = 2$. Let $u \in V(\Delta) \cap V(\Gamma_t)$ for some t , with $0 \leq t \leq k$. Since u has at most one neighbor in $V(\Gamma) \setminus V(\Gamma_t)$ and $k \geq 3$, there exists another vertex $v \in V(\Delta) \cap V(\Gamma_t)$ adjacent to u . Now, if w is any vertex of Δ other than u and v , then since w is adjacent to two vertices u and v of Γ_t it must belong to $V(\Gamma_t)$. Hence $V(\Delta) \subseteq V(\Gamma_t)$ and, consequently, $\Delta = \Gamma_t$.

Now, let $n \geq 3$. Note that $S(n - 1, k)$ is connected and has no bridges since every edge of $S(n - 1, k)$ lies on a cycle (which can be seen by induction on n). If $\Delta \neq \Gamma_i$ for $i = 0, \dots, k$, then Δ shares its vertices with at least two Γ_s and Γ_t . By the definition, exactly one extreme vertex, say u , of Γ_s is adjacent to exactly one extreme vertex, say v , of Γ_t . Because of the connectivity, Δ must contain the edge uv . Note that for any vertex w outside Γ_s and Γ_t , the distance between w and either u or v is greater than the diameter of $S(n - 1, k)$, and so $w \notin V(\Delta)$. It follows that Δ is a subgraph of $\Gamma' := \Gamma[V(\Gamma_s) \cup V(\Gamma_t)]$. However, uv is a bridge for Γ' and thus a bridge for Δ , a contradiction. \square

The following lemma reveals the structure of strongly Δ -partitioned Cayley graphs.

Lemma 4.4. *Let Γ be a Cayley graph with a subgraph Δ such that Γ is strongly Δ -partitioned. Then, the vertex sets of the copies of Δ are all the right cosets of a subgroup of the underlying group of Γ .*

Proof. Let Γ be a Cayley graph on a group G , and $X \subseteq G$ be such that $1 \in X$ and $\Gamma[X]$, the subgraph of Γ induced by X , is isomorphic to Δ . Since for any $x \in X$, $\Gamma[Xx^{-1}]$ is isomorphic to Δ and $1 \in Xx^{-1}$, from the hypothesis of the lemma, it follows that $Xx^{-1} = X$. Thus $XX^{-1} = X$ and, hence, X is a subgroup of G . As for any $g \in G$, $\Gamma[Xg]$ is isomorphic to Δ and the sets Xg cover all elements of G , it follows that the vertex set of every induced subgraph of Γ isomorphic to Δ is a right coset of X , as required. \square

Definition 4.5. Let Γ be a strongly Δ -partitioned graph. We say that Γ has *connection constant c* if there are exactly c edges between any two copies of Δ in Γ . We denote the set of all strongly Δ -partitioned graphs with connection constant c by $\mathcal{SP}_c(\Delta)$.

Remark 4.6. The family $\mathcal{SP}_1(K_d)$ contains only one regular graph. However, this is not the case in any regular graph Δ . If $\Gamma \in \mathcal{SP}_1(\Delta)$ is a regular graph with Δ being a d -regular graph on k vertices, then Γ necessarily contains $k + 1$ copies of Δ and thus Γ is $(d + 1)$ -regular with $k(k + 1)$ vertices. For instance, in the case in which Δ is C_4 , the cycle on 4 vertices, Γ is a cubic graph on 20 vertices. By a computer search, we found all the regular graphs in $\mathcal{SP}_1(C_4)$. It turned out that there are seven non-isomorphic such graphs, among which only one is a Cayley graph.

Here we recall some notions from group theory that will be used in what follows. Let G be a finite group and H be a nontrivial proper subgroup of G . The conjugate of H by an element g of G is defined as $H^g = \{h^g : h \in H\}$, where $h^g := g^{-1}hg$ denotes the conjugate of h by g . The group G is called a *Frobenius group* with *Frobenius complement H* if $H \cap H^g = \{1\}$ for all $g \in G \setminus H$. A celebrated theorem of Frobenius states that $N := G \setminus \bigcup_{g \in G} (H \setminus \{1\})^g$ is a normal subgroup of G , called the Frobenius kernel of G , satisfying $G = NH$ and $N \cap H = \{1\}$, that is, $G = N \rtimes H$ is a semidirect product of N by H (see [17, 8.5.5]). The other concepts we use in the following are standard and can be found in Robinson [17].

Theorem 4.7. *Suppose that Γ and Δ are two regular graphs and $\Gamma \in \mathcal{SP}_1(\Delta)$. If Γ is a Cayley graph $\text{Cay}(G, C)$, then $|\Delta| + 1 = p^m$ is a prime power, $G = N \rtimes H$ is a Frobenius group with minimal normal Frobenius kernel $N \cong \mathbb{Z}_p^m$ and Frobenius complement H , $C = C' \cup \{c\}$ with $\Delta \cong \text{Cay}(H, C')$ and $c^2 = 1$, and either*

- (i) $c \in N$ and $H = \langle C' \rangle$, or

(ii) $c = h^n$ for some $h \in H \setminus \{1\}$ and $n \in N \setminus \{1\}$, and $H = \langle C', h \rangle$.

Conversely, if Δ satisfies the above conditions, then $\text{Cay}(G, C) \in \mathcal{SP}_1(\Delta)$.

Proof. Let $\Gamma = \text{Cay}(G, C)$, and $\Delta_0, \Delta_1, \dots, \Delta_k$ be the copies of Δ in Γ . As there is exactly one edge between any two copies of Δ , it is observed that $|\Delta| = k$ and Γ is $(d+1)$ -regular if Δ is d -regular. Let $H := V(\Delta_0)$ and assume, without loss of generality, that $1 \in H$. By Lemma 4.4, H is a subgroup of G . Let C' be the neighborhood of 1 in $\Gamma[H]$. Since Γ is $(d+1)$ -regular, besides the elements of C' , the vertex 1 has exactly one other neighbor, say $c \in G \setminus H$. So $C = C' \cup \{c\}$. Since H is a subgroup of G , $C'^{-1} \subseteq H$, which implies that $C'^{-1} = C'$. Thus, $c = c^{-1}$ is an involution. Clearly, $Hc \neq H$ so that $\Gamma[Hc] = \Delta_i$ for some $1 \leq i \leq k$. On the other hand,

$$1 = |E(\Delta_0, \Delta_i)| = |\{\{h, ch\} : h \in H \cap H^c\}| = |H \cap H^c|,$$

from which it follows that $H \cap H^c = \{1\}$. Now, a simple verification shows that $Hch \cap Hch' = \emptyset$ for all distinct elements $h, h' \in H$. Since $\Gamma[H] = \Delta_0$ and $\Gamma[Hch]$ ($h \in H$) are equal to $\Delta_1, \dots, \Delta_k$ in some order, we must have

$$G = H \cup \bigcup_{h \in H} Hch,$$

where the unions are disjoint. As a result, every element $g \in G \setminus H$ can be written as $g = hch'$ for some $h, h' \in H$, from which it follows that

$$H \cap H^g = (H^{h'^{-1}} \cap (H^h)^c)^{h'} = (H \cap H^c)^{h'} = \{1\}^{h'} = \{1\}.$$

Hence, G is a Frobenius group with complement H . Let N be the Frobenius kernel of G . By [17, 10.5.1(i)], N is nilpotent. Let N_0 be a nontrivial characteristic subgroup of N with minimum order. Then N_0 is a normal subgroup of G (see [17, 1.5.6(iii)]). Note that N_0 is an elementary Abelian p -group for N_0 is nilpotent and the subgroup of N_0 generated by central elements of a given prime order p dividing $|Z(N_0)|$ is a characteristic subgroup of N_0 and hence of N (see [17, 1.5.6(ii)]). If $N \neq N_0$, then N_0H is a Frobenius group for N_0H is a subgroup of G and $H \cap H^g = 1$ for all $g \in N_0H \setminus H$. Moreover, as a proper subgroup of N , $|N_0| \leq |N|/2 \leq (k+1)/2$ and hence $|N_0| - 1$ is not divisible by $|H| = k$ contradicting [17, Exercises 8.5(6)]. Thus $N = N_0$ so that $k+1 = |N| = p^m$ is a prime power for some $m \geq 1$. Note that N is a minimal normal subgroup of G for if N contains a nontrivial normal subgroup N_0 of G properly, then N_0H would be a Frobenius group which leads us to the same contradiction as above. If $c \in N$, then since $G \subseteq N\langle C' \rangle$ it follows that $H = \langle C' \rangle$. Now assume that $c \notin N$. Then $c^n \in H \setminus \{1\}$ for some $n \in N \setminus \{1\}$. As $G \subseteq N\langle C', c^n \rangle$ it follows that $H = \langle C', c^n \rangle$, as required. The converse is straightforward. \square

We are now in a position to conclude the main result of this section.

Theorem 4.8. *The graph $S^{++}(n, k)$ is a Cayley graph if and only if either*

- (i) $n = 1$,
- (ii) $k \leq 2$, or

(iii) $n = 2$ and $k + 1 = p^m$ is a prime power.

Furthermore, in the case (iii), we have

$$S^{++}(n, k) \cong \text{Cay}(G, (H \setminus \{1\}) \cup \{c\}),$$

for every Frobenius group G with complement H of order $p^m - 1$, elementary Abelian minimal normal Frobenius kernel of order p^m , and involution $c \in G \setminus H$.

Proof. By Proposition 4.1, $S^{++}(n, k)$ for $n \geq 3$ and $k \geq 3$ is not a Cayley graph. As mentioned above, $S^{++}(n, 1)$, $S^{++}(n, 2)$, and $S^{++}(1, k)$ are all Cayley graphs. So, we may assume that $n = 2$ and $k \geq 3$.

First, we show that $S^{++}(2, q - 1)$ are Cayley graphs for all prime powers q . Let \mathbb{F}_q denote the finite field with q elements. Then $G := \mathbb{F}_q^* \times \mathbb{F}_q$ together with the multiplication

$$(x, a) \cdot (y, b) = (xy, xb + a),$$

forms a group known as *one dimensional affine group*. We show that $S^{++}(2, q - 1) \cong \text{Cay}(G, C)$, where $C = \{(x, 0) : 1 \neq x \in \mathbb{F}_q^*\} \cup \{(-1, -1)\}$. To this end, let $H := \{(x, 0) : x \in \mathbb{F}_q^*\}$ be a subgroup of G of order $q - 1$. Then H has q right cosets each of which induces a complete subgraph in $\text{Cay}(G, C)$ for $h'g(hg)^{-1} = h'h^{-1} \in C$ for all distinct elements hg and $h'g$ of a right coset Hg of H . Since $(x, 0)(1, ax^{-1}) = (x, a)$ covers all elements of G when x and a ranges over \mathbb{F}_q^* and \mathbb{F}_q , respectively, it follows that every right coset of H has a representative of the form $(1, b)$ for some $b \in \mathbb{F}_q$. Let Hg and Hg' be distinct right cosets of H with $g = (1, a)$ and $g' = (1, a')$. Then an element hg of Hg is adjacent to an element $h'g'$ of Hg' if and only if $h'g'g^{-1}h^{-1} = (h'g')(hg)^{-1} \in C$ or equivalently $(h'g')(hg)^{-1} = (-1, -1)$ as $g'g^{-1} \notin H$. A simple verification shows that this equation has a unique solution for (h, h') so that there is a unique edge between any two right cosets of H . Indeed, $h = (x, 0)$ and $h' = (x', 0)$ satisfy the equation if and only if $-x' = x = (a' - a)^{-1}$. Hence, from the definition, it follows that $S^{++}(2, q - 1) \cong \text{Cay}(G, C)$.

Now, assume that $\Gamma := S^{++}(2, k) \cong \text{Cay}(G, C)$ be a presentation of $S^{++}(2, k)$ as a Cayley graph. By Proposition 4.3, Γ is strongly Γ_0 -partitioned for some complete subgraph Γ_0 of Γ of order k . Let $H := V(\Gamma_0)$ and assume that $1 \in H$. We know from Lemma 4.4 that H is a subgroup of G . By Theorem 4.7, $k + 1 = p^m$ is a prime power, $G = N \rtimes H$ is a Frobenius group with Frobenius kernel N and Frobenius complement H such that $N \cong \mathbb{Z}_p^m$ is a minimal normal subgroup of G , $C = C' \cup \{c\}$, $C'^{-1} = C' \subseteq H$, $c^2 = 1$, and either

- (a) $c \in N$ and $H = \langle C' \rangle$, or
- (b) $c = h^n$ for some $h \in H \setminus \{1\}$ and $n \in N \setminus \{1\}$, and $H = \langle C', h \rangle$.

Since Γ_0 is a complete graph, we must have $H \setminus \{1\} \subseteq C$. Then, (a) and (b) together are equivalent to say that $c \in G \setminus H$. The proof is now complete. □

As a generalization of Theorem 4.7, we pose the following problem.

Problem 4.9. Let Δ be a regular graph. Classify all Cayley graphs in $\mathcal{SP}_c(\Delta)$ for $c \geq 2$.

5 New non-Cayley numbers

In this final section, we give a partial answer to a famous rather old open problem in algebraic graph theory. A positive integer n is called a *Cayley number* if all vertex-transitive graphs of order n are Cayley graphs. Marušič [11] in 1983 posed the problem of characterizing the set \mathcal{NC} of all non-Cayley numbers. Since disjoint unions of copies of vertex-transitive (non-Cayley) graphs are again vertex-transitive (non-Cayley) graphs, it follows that every multiple of a non-Cayley number is again a non-Cayley number. Hence the problem of determining \mathcal{NC} reduces to finding ‘minimal’ non-Cayley numbers. It is well-known that all primes are Cayley numbers. Following a series of papers by various authors, McKay and Praeger [13] and Iranmanesh and Praeger [7] provided necessary and sufficient conditions under which the product of two and three distinct primes is a Cayley number, respectively. In the same paper, McKay and Praeger established the following remarkable result determining all non-square-free Cayley numbers.

Theorem 5.1 (McKay and Praeger [13]). *Let n be a positive integer that is divisible by the square of a prime p . Then $n \in \mathcal{NC}$ unless $n = p^2$, $n = p^3$, or $n = 12$.*

It follows that, for determining \mathcal{NC} , it is enough to consider only square-free positive integers. While the problem is yet open for the products of at least four distinct primes, there are partial results worth to mention here.

Theorem 5.2 (Dobson and Spiga [3]). *There exists an infinite set of primes every finite product of its distinct elements is a Cayley number.*

As a consequence of Theorem 4.8, the graph $S^{++}(2, k)$ that has $k(k + 1)$ vertices is not a Cayley graph if $k + 1$ is not a prime power. Therefore, we obtain a new infinite class of square-free non-Cayley numbers as follows.

Theorem 5.3. *Let k be any positive integer such that $k(k + 1)$ is square-free, and $k + 1$ is not a prime. Then, $k(k + 1) \in \mathcal{NC}$.*

As mentioned in Dobson and Spiga [3], it is straightforward by making use of the group-theoretic and the number-theoretic results already available in the literature to prove that Cayley numbers have density zero in the set of natural numbers, and hence the density of non-Cayley numbers is 1. In the light of this fact, one might wonder about the distribution of the numbers k satisfying the conditions of Theorem 5.3 in the set of positive integers. The following theorem shows that for large enough N , more than one third of positive integers less than or equal to N satisfies the conditions of Theorem 5.3.

Theorem 5.4. *The density of the set*

$$\{k : k(k + 1) \text{ is square-free, and } k + 1 \text{ is not a prime}\}$$

is about 0.3226.

Proof. Let $f \in \mathbb{Z}[t]$ be a primitive polynomial (that is, the greatest common divisor of its coefficients is 1) without multiple roots such that its image on \mathbb{N} has k -free greatest common divisor. Recall that a number that is not divisible by any proper k -th power is called k -free. Let $S_f^k(x)$ denote the number of all positive integers $n \leq x$ such that $f(n)$ is k -free, and consider

$$\delta_{f,k} := \prod_{p \text{ prime}} \left(1 - \frac{\varrho(p^k)}{p^k} \right),$$

where $\varrho(d)$ denotes the number of roots of f in \mathbb{Z}_d . Ricci [16] (see also Pappalardi [14]) proved that

$$\mathcal{S}_f^k(x) \sim \delta_{f,k} x$$

provided that $\deg f \leq k$. Clearly, the function $f(t) := t(t+1)$ satisfies the above requirements of Ricci's theorem for $k = 2$. Also, it is obvious that $\varrho(p^2) = 2$ for all primes p . Thus, by Ricci's theorem, the density of all positive integers k , for which $k(k+1)$ is square-free, in the set of all positive integers, is equal to

$$\delta_{f,2} = \prod_{p \text{ prime}} \left(1 - \frac{2}{p^2}\right) = 2C_{\text{Feller-Tornier}} - 1 \approx 0.3226340989,$$

where $C_{\text{Feller-Tornier}}$ is the Feller-Tornier constant (see Finch [4, §2.4.1]). Since primes have zero density in the set of all positive integers, the result follows. \square





To date, all the numbers whose membership in \mathcal{NC} is known are determined based on the results of [7, 12, 13]. Using a computer search, we see that the list of the numbers whose membership in \mathcal{NC} is not yet determined begins with

9982, 12958, 18998, 19646, 20398, 21574, 24662, 25438, 25606, ...

A simple computation reveals that among the numbers less than or equal to 10^8 , there are 2763 square-free integers of the form $k(k+1)$, with $k+1$ not a prime of which the following eight integers are new non-Cayley numbers:

1386506, 2668322, 15503906, 23985506, 38359442, 74261306, 89898842, 95912642.

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The chromatic index of strongly regular graphs

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Abstract

We determine (partly by computer search) the chromatic index (edge-chromatic number) of many strongly regular graphs (SRGs), including the SRGs of degree $k \leq 18$ and their complements, the Latin square graphs and their complements, and the triangular graphs and their complements. Moreover, using a recent result of Ferber and Jain, we prove that an SRG of even order n , which is not the block graph of a Steiner 2-design or its complement, has chromatic index k , when n is big enough. Except for the Petersen graph, all investigated connected SRGs of even order have chromatic index equal to k , i.e., they are class 1, and we conjecture that this is the case for all connected SRGs of even order.

Keywords: Strongly regular graph, chromatic index, edge coloring, 1-factorization.

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1 Introduction

An *edge-coloring* of a graph G is a coloring of its edges such that intersecting edges have different colors. Thus a set of edges with the same colors (called a color class) is a matching. The *edge-chromatic number* $\chi'(G)$ (also known as the *chromatic index*) of G is the

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minimum number of colors in an edge-coloring. By Vizing's famous theorem [24], the chromatic index of a graph G of maximum degree Δ is Δ or $\Delta + 1$. A graph with maximum degree Δ is called class 1 if $\chi'(G) = \Delta$ and is called class 2 if $\chi'(G) = \Delta + 1$. It is also known that determining whether a graph G is class 1 is an NP-complete problem [18]. If G is regular of degree k , then G is class 1 if and only if G has an edge coloring such that each color class is a perfect matching. A perfect matching is also called a *1-factor*, and a partition of the edge set into perfect matchings is called a *1-factorization*. So being regular and class 1 is the same as having a 1-factorization (being 1-factorable), and requires that the graph has even order.

A graph G is called a *strongly regular graph* (SRG) with parameters (n, k, λ, μ) if it has n vertices, is k -regular ($0 < k < n - 1$), any two adjacent vertices of G have exactly λ common neighbors and any two distinct non-adjacent vertices of G have exactly μ common neighbors. The complement of a strongly regular graph with parameters (n, k, λ, μ) is again strongly regular, and has parameters $(n, n - k - 1, n - 2k + \mu - 2, n - 2k + \lambda)$. An SRG G is called *imprimitive* if G or its complement is disconnected, and *primitive* otherwise. A disconnected SRG is ℓK_m ($\ell, m \geq 2$), the disjoint union of ℓ cliques of order m (indeed, $\mu = 0$ implies that no two vertices have distance two, so every connected component is a clique). It is well-known that K_m ($m \geq 2$), and hence also ℓK_m , is class 1 if and only if m is even. The complement of ℓK_m is a regular complete multipartite graph which is known to be class 1 if and only if the order is even [17].

A *vertex coloring* of G is a coloring of the vertices of G such that adjacent vertices have different colors. The *chromatic number* $\chi(G)$ of G is the minimum number of colors in a vertex coloring. For the chromatic number there exist bounds in terms of the eigenvalues of the adjacency matrix, which turn out to be especially useful for strongly regular graphs (see for example [6]). These bounds imply that there exist only finitely many primitive SRGs with a given chromatic number, and made it possible to determine all SRGs with chromatic number at most four (see [15]). Motivated by these results, Alex Rosá asked the third author whether eigenvalue techniques can give information on the chromatic index of an SRG. There exist useful spectral conditions for the existence of a perfect matching (see [5, 9]), and Brouwer and Haemers [5] have shown that every regular graph of even order, degree k and second largest eigenvalue ϑ_2 contains at least $\lfloor (k - \vartheta_2 + 1)/2 \rfloor$ edge disjoint perfect matchings. From this it follows that every connected SRG of even order has a perfect matching. Moreover, Cioabă and Li [10] proved that any matching of order $k/4$ of a primitive SRG of valency k and even order, is contained in a perfect matching. These authors conjectured that $k/4$ can be replaced by $\lceil k/2 \rceil - 1$ which would be best possible. Unfortunately, we found no useful eigenvalue tools for determining the chromatic index. However, the following recent result of Ferber and Jain [13] gives an asymptotic condition for being class 1 in terms of the eigenvalues.

Theorem 1.1. *There exist universal constants n_0 and k_0 , such that the following holds. If G is a connected k -regular graph of even order n with eigenvalues $k = \vartheta_1 > \vartheta_2 \geq \dots \geq \vartheta_n$, and $n > n_0$, $k > k_0$ and $\max\{\vartheta_2, -\vartheta_n\} < k^{0.9}$, then G is class 1.*

If the maximum distance in G is 2 (as is the case for a connected SRG), then $n \leq 1 + k + k(k - 1) = k^2 + 1$. This implies that for an SRG we do not need to require that $k > k_0$ when we take $n_0 \geq k_0^2 + 1$. Theorem 1.1 enables us to show that, except for one family of SRGs, all connected SRGs of even order n are class 1, provided n is large enough. In addition, we present a number of sufficient conditions for an SRG to be class 1.

By computer, using SageMath [22], we verified that all primitive SRGs of even order and degree $k \leq 18$ and their complements are class 1, except for the Petersen graph, which has parameters $(10, 3, 0, 1)$ and edge-chromatic number 4 (see [20, 25] for example). We also determine the chromatic index of several other primitive SRGs of even order, and all are class 1. Therefore we believe:

Conjecture 1.2. *Except for the Petersen graph, every connected SRG of even order is class 1.*

2 Sufficient conditions for being class 1

A well known conjecture (first stated by Chetwynd and Hilton [8], but attributed to Dirac) states that every k -regular graph of even order n with $k \geq n/2$ is 1-factorable. Cariolaro and Hilton [7] proved that the conclusion holds when $k \geq 0.823n$, and Csaba, Kühn, Lo, Osthus, and Treglown [11], proved the following result.

Theorem 2.1. *There exists a universal constant n_0 , such that if n is even, $n > n_0$ and if $k \geq 2\lceil n/4 \rceil - 1$, then every k -regular graph of order n has chromatic index k .*

König [19] proved that every regular bipartite graph of positive degree has a 1-factorization. We need the following generalization of König’s result.

Lemma 2.2. *Let $G = (V, E)$ be a connected regular graph of even order n , and let $\{V_1, V_2\}$ be a partition of V such that $|V_1| = |V_2| = n/2$.*

- (i) *If the graphs induced by V_1 and V_2 are 1-factorable, then so is G .*
- (ii) *If V_1 (and hence V_2) is a clique or a coclique, then G is class 1.*

Proof. Partition the edge set E into two classes E_1 and E_2 , where E_1 contains all edges with both endpoints in the same vertex set V_1 or V_2 , and the edges of E_2 have one endpoint in V_1 and the other endpoint in V_2 .

(i): If the graphs induced by V_1 and V_2 are 1-factorable, then both have the same degree, and therefore also (V, E_1) is 1-factorable. By König’s theorem (V, E_2) is 1-factorable, therefore G is class 1.

(ii): If V_1 is a coclique, then so is V_2 and we have the theorem of König. If V_1 is a clique, then so is V_2 . If $n/2$ is even, then the result is proved in (i). If $n/2$ is odd, then we choose a 1-factor F in (V, E_2) (here we use that G is connected), and define $E'_2 = E_2 \setminus F$ and $E'_1 = E_1 \cup F$. Then (V, E'_2) is 1-factorable (or has no edges), and (V, E'_1) consists of two cliques of order $n/2$ and the 1-factor F . Thus F gives a bijection ϕ (say) between V_1 and V_2 . By Vizing’s theorem the edges of both cliques can be colored with $n/2$ colors. We do this coloring such that ϕ preserves colors, which means that $\{v, w\}$ and $\{\phi(v), \phi(w)\}$ get the same color. Then for each edge $\{v, \phi(v)\}$ of F , the two sets of colored edges that intersect at v and $\phi(v)$ use the same $n/2 - 1$ colors. So we can color $\{v, \phi(v)\}$ with the remaining color. □

There exist several SRGs that have the partition of case (i). The Gewirtz graph is the unique SRG with parameters $(56, 10, 0, 2)$, and admits a partition into two Coxeter graphs (see [4]). The Coxeter graph is known to be 1-factorable (see [3]), therefore the Gewirtz graph is class 1. The same holds for the point graph of the generalized quadrangle $\text{GQ}(3, 9)$ (the unique SRG $(112, 30, 2, 10)$), which admits a partition into two Gewirtz graphs, and for

the Higman-Sims graph (the unique $\text{SRG}(100, 22, 0, 6)$), which can be partitioned into two copies of the Hoffman-Singleton graph (the unique strongly regular graph with parameters $(50, 7, 0, 1)$), which has chromatic index 7 (see Section 4).

Suppose $\vartheta_1 \geq \vartheta_2 \geq \dots \geq \vartheta_n$ are the eigenvalues of a graph G of order n . Hoffman (see [6, Theorem 3.6.2] for example) proved that the chromatic number of G is at least $1 - \vartheta_1/\vartheta_n$. A vertex coloring that meets this bound is called a *Hoffman coloring*. For k -regular graphs, the color classes of a Hoffman coloring are cocliques of which the size meets Hoffman's coclique bound $n\vartheta_n/(\vartheta_n - k)$. This implies (see [6] for example) that all the color classes have equal size, and any vertex v of G has exactly $-\vartheta_n$ neighbors in each color class different from the color class of v .

Theorem 2.3. *Suppose $G = (V, E)$ is a k -regular graph with an even chromatic number $2t$ (say) that meets Hoffman's bound. Then both G and its complement \overline{G} are class 1, or \overline{G} is a disjoint union of cliques of odd order.*

Proof. Let S_1, \dots, S_{2t} be the color classes in a Hoffman coloring of G . Since G is regular, this implies that each S_i is a coclique attaining equality in the Hoffman ratio bound, which means that each vertex outside S_i has exactly $-\vartheta_n$ neighbors in S_i . Hence, each subgraph induced by two distinct cocliques S_i and S_j is a bipartite regular graph of valency $-\vartheta_n$. A 1-factorization of K_{2t} corresponds to a partition E_1, \dots, E_{2t-1} of E , such that each (V, E_i) consists of t disjoint regular bipartite graphs of degree $-\vartheta_n = k/(2t - 1)$. By König's theorem it follows that each (V, E_i) is 1-factorable, and therefore G is class 1.

For the complement $\overline{G} = (V, F)$ of G , a similar approach works. We can partition the edge set F into the subsets $F_0, F_1, \dots, F_{2t-1}$, such that for $i = 1, \dots, 2t - 1$ the graph (V, F_i) is the disjoint union of t regular bipartite graphs of the same positive degree (if the degree is 0, then \overline{G} is a disjoint union of cliques). But now there is an additional graph (V, F_0) consisting of $2t$ disjoint cliques. We combine F_0 and F_1 . Then $(V, F_0 \cup F_1)$ is the disjoint union of t complements of regular incomplete bipartite graphs with the same positive degree, and therefore has a 1-factorization by Lemma 2.2. Since (V, F_i) has a 1-factorization for $i = 2, \dots, 2t - 1$, it follows that \overline{G} is 1-factorable. \square

For an SRG the color partition of a Hoffman coloring corresponds to a so-called *spread* in the complement (see [16]). As a consequence of this result, it follows that any primitive strongly regular graph with a spread with an even number of cliques, or a Hoffman coloring with an even number of colors is class 1. Among such SRGs are the Latin square graphs. Consider a set of t ($t \geq 0$) mutually orthogonal Latin squares of order m ($m \geq 2$). The vertices of the Latin square graph are the m^2 entries of the Latin squares, and two distinct entries are adjacent if they lie in the same row, the same column, or have the same symbol in one of the squares. If $t = m - 1$ we obtain the complete graph K_{m^2} , and if $t = m - 2$ we have a complete multipartite graph. Otherwise the Latin square graph is a primitive SRG with parameters $(m^2, (t + 2)(m - 1), m - 2 + t(t + 1), (t + 1)(t + 2))$. If $t = 0$ we only have the rows and columns, then the Latin square graph is better known as the Lattice graph $L(m)$. If $m \neq 4$, the Lattice graph is determined by the parameters. The m rows of a Latin square give a partition of the vertex set of the Latin square graph into cliques, which is a spread. Thus we have:

Corollary 2.4. *If G is a Latin square graph of even order, then both G and its complement are 1-factorable.*

3 Asymptotic results

A Steiner 2-design (or $2-(m, \ell, 1)$ design) consists of a point set \mathcal{P} of cardinality m , together with a collection of subsets of \mathcal{P} of size ℓ ($\ell \geq 2$), called *blocks*, such that every pair of points from \mathcal{P} is contained in exactly one of the blocks. The *block graph* of a Steiner 2-design is defined as follows. The blocks are the vertices, and two vertices are adjacent if the blocks intersect in one point. If $m = \ell^2 - \ell + 1$, the Steiner 2-design is a projective plane, and the block graph is K_m . Otherwise the block graph is an SRG with parameters $(m(m-1)/\ell(\ell-1), \ell(m-\ell)/(\ell-1), (\ell-1)^2 + (m-2\ell+1)/(\ell-1), \ell^2)$.

Theorem 3.1. *There exists an integer n_0 , such that every primitive strongly regular graph of even order $n > n_0$, which is not the block graph of a Steiner 2-design or its complement, is class 1.*

Proof. Suppose G is a primitive (n, k, λ, μ) -SRG of even order n . Then it is well-known (see for example [6, Chapter 9]) that G has exactly three distinct eigenvalues $k = \vartheta_1$, ϑ_2 and ϑ_n . Moreover, the eigenvalues are nonzero integers and satisfy $k + \vartheta_2\vartheta_n = \mu$. Assume that G nor its complement \overline{G} is the block graph of a Steiner 2-design or a Latin square graph. Using a result of Neumaier [21] (known as the claw bound), we get that

$$\vartheta_2 \leq \vartheta_n(\vartheta_n + 1)(\mu + 1)/2 - 1.$$

Another result of Neumaier [21] (the μ -bound) gives $\mu \leq \vartheta_n^3(2\vartheta_n + 3)$. Combining these inequalities, after some straightforward calculations, we obtain that $\vartheta_2 < (-\vartheta_n)^6$. Since $k + \vartheta_2\vartheta_n = \mu > 0$, we deduce that

$$k^6 > (-\vartheta_2\vartheta_n)^6 > \vartheta_2^6\vartheta_n^6 = \vartheta_2^7, \quad \text{so} \quad \vartheta_2 < k^{6/7}.$$

Next we apply the same result to \overline{G} , and obtain $-1 - \vartheta_n < (1 + \vartheta_2)^6$, which yields $-\vartheta_n \leq (2\vartheta_2)^6$ (since ϑ_2 is a positive integer). Hence

$$k^6 > (-\vartheta_2\vartheta_n)^6 > 2^{-6}(-\vartheta_n)(-\vartheta_n)^6 = 2^{-6}(-\vartheta_n)^7, \quad \text{so} \quad -\vartheta_n < (2k)^{6/7} < k^{0.9},$$

when k is large enough. Thus we get $\max\{\vartheta_2, -\vartheta_n\} \leq k^{0.9}$. Now we apply the result of Ferber and Jain and conclude that G is class 1 when n is large enough.

If G is a Latin square graph of even order then by Corollary 2.4 both G and its complement \overline{G} are class 1. □

In many cases the complement of the block graph of a Steiner 2-design has $k > n/2$, so it will have a 1-factorization by Theorem 2.1, provided n is even and large enough. The following result follows straightforwardly from the mentioned result of Cariolaro and Hilton [7].

Proposition 3.2. *If G is the complement of the block graph of a $2-(m, \ell, 1)$ design with $6\ell^2 \leq m$, then G is class 1, provided G has even order.*

For every $m \geq 2$ there is a unique $2-(m, 2, 1)$ design, and its block graph is the triangular graph $T(m)$. It is isomorphic to the line graph of the complete graph K_m , and if $m \geq 4$ $T(m)$ is an SRG with parameters $(m(m-1)/2, 2(m-2), m-2, 4)$. The triangular graph is uniquely determined by its parameters if $m \neq 8$. Alspach [1] has proved that $T(m)$ has

a 1-factorization if the order is even, which is the case if $m \equiv 0, \text{ or } 1 \pmod{4}$. Proposition 3.2 implies that the complement of $T(m)$ is class 1 if $m \geq 24$ and the order is even. The complement of $T(5)$ is the Petersen graph, which is class 2. For $5 < m < 24$ and $m \equiv 0, \text{ or } 1 \pmod{4}$ we found a 1-factorization in the complement of $T(m)$ by computer (see next section for more about the computer search). Thus we can conclude:

Theorem 3.3. *For $m \equiv 0, \text{ or } 1 \pmod{4}$ the triangular graph $T(m)$ is class 1, and if $m \neq 5$ so is its complement.*

If the block size equals 3, the design is better known as a Steiner triple system. The chromatic index of the block graph of a Steiner triple system is investigated in [12]. The paper contains several sufficient conditions for such a graph to be class 1, and the authors conjecture that all these graphs are class 1 when the order is even. One of the results from [12] (Theorem 2.2) can be generalized to arbitrary Steiner 2-designs. A set of m/ℓ disjoint blocks of a $2-(m, \ell, 1)$ design is called a *parallel class*, and a partition of the block graph into parallel classes is a *parallelism*. A parallelism of a Steiner 2-design gives a Hoffman coloring in the block graph, so we have:

Proposition 3.4. *If a Steiner 2-design has a parallelism with an even number of parallel classes, then the block graph and its complement are class 1.*

4 SRGs of degree at most 18

According to the list of Brouwer [2] all primitive SRGs of even order and degree at most 18 are known (one only has to check the parameter sets up to $n = 18^2 + 1 = 325$). The parameters together with the number of nonisomorphic SRGs with $k < n/2$ are given in Table 1 (the ones with $k \geq n/2$ are the complements of a to e). The graph with parameter

Table 1: Primitive SRGs with n even and $k \leq 18, k < n/2$.

a	(10, 3, 0, 1)	1	f	(36, 10, 4, 2)	1	k	(50, 7, 0, 1)	1
b	(16, 5, 0, 2)	1	g	(36, 14, 4, 6)	180	l	(56, 10, 0, 2)	1
c	(16, 6, 2, 2)	2	h	(36, 14, 7, 4)	1	m	(64, 14, 6, 2)	1
d	(26, 10, 3, 4)	10	i	(36, 15, 6, 6)	32548	n	(64, 18, 2, 6)	167
e	(28, 12, 6, 4)	4	j	(40, 12, 2, 4)	28	o	(100, 18, 8, 2)	1

set a is the Petersen graph, which is class 2. The complement of the Petersen graph is the triangular graph $T(5)$ which is class 1 by Alspach’s result [1]. Also Case h and one of the graphs of Case e is a triangular graph and therefore class 1. For the parameter sets f, m and o there is a unique SRG, the so called Lattice graph. This SRG belongs to the Latin square graphs, and by Corollary 2.4 the graph is class 1, and so is its complement. Case l is the Gewirtz graph, which is class 1 by Lemma 2.2, as we saw in Section 2. All other graphs are tested by computer (we actually tested all graphs in Table 1 and their complements). Using SageMath [22], we wrote a computer program that searches for an edge coloring in a k -regular graph with k colors. In each step we look (randomly) for a perfect matching, remove all its edges and continue until the remaining graph has no perfect matching. If there are still edges left we start again. We run this algorithm repeatedly until an edge coloring is found. The code for this project is made freely available in a public GitHub repository which can be found at [14]. By use of this approach we found a 1-factorization

in all graphs of Table 1, and in their complements, except for the Petersen graph. Thus we found:

Theorem 4.1. *With the single exception of the Petersen graph, a primitive SRG of even order and degree at most 18 is class 1 and so is its complement.*


For the description of the graphs we used the website of Spence [23]. This website also contains several SRGs with parameters $(50, 21, 8, 9)$. We also ran the search for these graphs. All are class 1.

It is surprising that in all cases our straightforward heuristic finds a 1-factorization. The heuristic is fast. It took about one hour to find a 1-factorization in each of the 32548 SRGs with parameter set i .

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A simple and elementary proof of Whitney's unique embedding theorem

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Abstract

In this note we give a short and elementary proof of a more general version of Whitney's theorem that 3-connected planar graphs have a unique embedding in the plane. A consequence of the theorem is also that cubic plane graphs cannot be embedded in a higher genus with a simple dual. The aim of this paper is to promote a simple and elementary proof, which is especially well suited for lectures presenting Whitney's theorem.

Keywords: Polyhedra, graph, embedding.

Math. Subj. Class. (2020): 05C10, 57M60, 57M15

1 Introduction

Whitney's famous unique embedding theorem has been formulated in various equivalent forms. One form is that the facial cycles of 3-connected graphs embedded in the plane are well determined, so that for any two embeddings there is a graph isomorphism between the duals. Another is (implied by the Jordan-Schönflies Theorem) that any two topological embeddings of a graph on the sphere can be mapped onto each other by a homeomorphism of the sphere that maps the two images of a vertex onto each other.

We will formulate the theorem and describe the proof in the language of combinatorial embeddings in oriented closed surfaces. For the translation to the language of topological 2-cell embeddings, methods from standard books like [1] or [3] can be used.

We interpret each edge $\{u, v\}$ of an undirected embedded graph G as two directed edges: $e = (u, v)$ and its inverse $e^{-1} = (v, u)$. An embedded graph in an oriented closed surface is a graph where for every vertex u there is a cyclic order of all edges (u, \cdot) (usually called a *rotation*). The cyclic ordering defines the orientation around the vertex. We write

*I would like to thank Bojan Mohar for pointing me to the earlier uses of the crossing Jordan curves argument!
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$\text{nx}(e)$ for the next edge in the order around the starting point of a directed edge e . The inverse graph or mirror image is the graph G^{-1} with all cyclic orders reversed.

A face in an embedded graph G is a directed cyclic walk e_0, \dots, e_{n-1} , so that for $0 \leq i < n$ we have that $\text{nx}(e_i^{-1}) = e_{(i+1) \pmod n}$. We say that the set $\{e, \text{nx}(e)\}$ forms an *angle* of G and G^{-1} if one of them has a face containing $e^{-1}, \text{nx}(e)$ as a subsequence. In this case the other has a face containing $\text{nx}(e)^{-1}, e$. If a face is a simple cyclic walk, we call the corresponding undirected cycle also a (simple) facial cycle. We consider an embedded graph G and its mirror image G^{-1} as equivalent, as the faces have the same sequences of underlying undirected edges – only in reversed order. The genus of an embedded graph can be computed by the Euler formula using the number v of vertices, e of (undirected) edges, and f of faces as $\gamma(G) = \frac{2-(v-e+f)}{2}$. We refer to a (not necessarily embedded) graph that can be embedded with genus 0 as planar and to an embedded graph with genus 0 as plane.

With this notation and concept of equivalence Whitney’s famous theorem [5] can be shortly stated as:

A 3-connected planar graph has an – up to equivalence – unique embedding in the plane.

We will prove a stronger theorem using the concept of *polyhedral embedding* that requires some important properties of polyhedra – that is plane 3-connected graphs – but allows higher genera. It is an easy consequence of the Jordan Curve Theorem that polyhedra are polyhedral embeddings.

Definition 1.1. A polyhedral embedding of a graph $G = (V, E)$ in an oriented closed surface is an embedding so that each facial walk is a simple cycle and the intersection of any two faces is either empty, a single vertex or a single edge.

For cubic embedded graphs this is equivalent to the dual graph being simple.

The argument of crossing Jordan curves that we will use in the proof was first published by Thomassen in [4], but also known to Robertson and later used by Mohar and Robertson in [2]. See also Theorem 5.7.1 in [3]. In fact, in [4] the argument was used to prove that 3-connected planar graphs embedded with genus $g > 0$ have facewidth at most 2. Together with Whitney’s theorem, this implies Theorem 1.2. We will give every detail of the proof in order to make it well suited for lectures presenting Whitney’s theorem, but the arguments are exactly the same arguments of crossing Jordan curves that Thomassen used – only that here the planar case, that is: Whitney’s theorem – is included too.

Theorem 1.2. *A 3-connected planar graph has an – up to equivalence – unique polyhedral embedding.*

Proof. Let G be a plane embedding of a 3-connected planar graph with mirror image G^{-1} and let G' be an embedding different from these two. We say that a vertex of G' has type 1 if the order is the same as in G , type -1 if it is the same as in G^{-1} and type 2 otherwise. As G' is neither G nor G^{-1} , G' has a vertex of type 2 or an edge with one vertex of type 1 and one vertex of type -1 .

Assume first that there is a vertex v of type 2. Let e_0, \dots, e_{d-1} be the order of edges around v in G' . If $\{e_0, e_1\}$ is not an angle of G , we take this set of edges. Otherwise assume w.l.o.g. that $e_1 = \text{nx}(e_0)$ in G and let j be minimal so that in G we have $\text{nx}(e_j) \neq e_{(j+1) \pmod d}$. As in G^{-1} we have $\text{nx}(e_j) = e_{j-1}$, the edge $e_{(j+1) \pmod d}$ follows e_j neither in G nor in G' , so $\{e_j, e_{(j+1) \pmod d}\}$ is not an angle in G . W.l.o.g. assume $j = 0$.

So the order around v in G is $e_0, e_{i_1}, \dots, e_{i_j}, e_1, e_{i_{j+1}}, \dots, e_{i_{d-2}}$ with $1 \leq j < d-2$ and assume w.l.o.g. that $e_{d-1} \in \{e_{i_{j+1}}, \dots, e_{i_{d-2}}\}$. Let $y = \max\{i_1, \dots, i_j\}$, so $y < d-1$ and $(y+1) \in \{i_{j+1}, \dots, i_{d-2}\}$, which implies that $\{e_y, e_{y+1}\}$ is an angle of G' with $e_y \in \{e_{i_1}, \dots, e_{i_j}\}$ and $e_{y+1} \in \{e_{i_{j+1}}, \dots, e_{i_{d-2}}\}$. Let F be the facial cycle in G' containing the angle $\{e_0, e_1\}$ and F' be the facial cycle containing $\{e_y, e_{y+1}\}$. We have $F \neq F'$ as otherwise the faces would not be simple cycles. In G these cycles are not facial cycles, but two Jordan curves crossing each other in v . Due to the Jordan curve theorem, there must be a second crossing, so F, F' are two facial cycles that have at least two vertices in common that are not endpoints of a common edge – a contradiction to G' being polyhedral.


Assume now that all vertices are of type 1 or type -1 . Then there is an edge e_0 with one vertex of type 1 and one of type -1 . Assume that in G the orientation around the type 1 vertex of e_0 is e_0, e_1, \dots, e_d and around the type -1 vertex it is $e_0^{-1}, e'_1, \dots, e'_d$, so in G' it is e_0, e_1, \dots, e_d resp. $e'_d, e'_{d-1}, \dots, e_0^{-1}$. In G' there is a face F containing e_d^{-1}, e_0, e'_d and another face F' containing e_1^{-1}, e_0^{-1}, e_1 . In G the corresponding cycles are again no facial cycles but Jordan curves crossing each other (with one common edge), so like in the first case we get a contradiction from the fact that there must be a second intersection between F and F' . \square

As plane embeddings of 3-connected graphs are all polyhedral, this also implies Whitney's theorem, but there are also other consequences that are worth mentioning. They follow already from Theorem 8.1 in [4]. Note that for graphs with 1- or 2-cut there are no polyhedral embeddings in any closed orientable surface.

Corollary 1.3.

- *There are no polyhedral embeddings of planar graphs in any orientable surface but the plane.*
- *There are no embeddings of cubic planar graphs with a simple dual in any orientable surface but the plane.*

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The average genus for bouquets of circles and dipoles

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Abstract

The bouquet of circles B_n and dipole graph D_n are two important classes of graphs in topological graph theory. For $n \geq 1$, we give an explicit formula for the average genus $\gamma_{\text{avg}}(B_n)$ of B_n . By this expression, one easily sees $\gamma_{\text{avg}}(B_n) = \frac{n - \ln n - \gamma + 1 - \ln 2}{2} + o(1)$, where γ is the *Euler-Mascheroni constant*. Similar results are obtained for D_n . Our method mainly depends on the technique of generating series and the knowledge in ordinary differential equations.

Keywords: Average genus, bouquet of circles, dipole, ordinary differential equation.

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1 Introduction and main results

A graph $G = (V(G), E(G))$ is permitted to have both loops and multiple edges. An embedding of a graph G into an orientable surface O_k is a *cellular embedding*, i.e., the interior of every face is homeomorphic to an open disc. The subscript in O_k is the genus of the orientable surface O_k , for $k \geq 0$. We denote the number of cellular embeddings of G on the surface O_k by $g_k(G)$, where, by the *number of embeddings*, we mean the number of equivalence classes under ambient isotopy. The *genus polynomial* of a graph G is given by

$$\Gamma_G(x) = \sum_{k \geq 0} g_k(G)x^k.$$

This sequence $\{g_k(G), k = 0, 1, 2, \dots\}$ is called the *genus distribution* of the graph G . For a graph G , it is well known that the total number of cellular embeddings is $\prod_{v \in V(G)} (d_G(v) - 1)!$, where $d_G(v)$ is the degree of the vertex v in G . For example, see [13, Chapter 3]. Hence,

$$\Gamma_G(1) = \sum_{k \geq 0} g_k(G) = \prod_{v \in V(G)} (d_G(v) - 1)! \tag{1.1}$$

The *average genus* $\gamma_{\text{avg}}(G)$ of the graph G is the expected value of the genus random variable, over all labeled 2-cell orientable embeddings of G , using the uniform distribution. In other words, the average genus of G is

$$\gamma_{\text{avg}}(G) = \frac{\Gamma'_G(1)}{\Gamma_G(1)} = \sum_{k=0}^{\infty} k \cdot \frac{g_k(G)}{\Gamma_G(1)}.$$

The study of the average genus of a graph began by Gross and Furst [9], and was much further developed by Chen and Gross [1, 2, 3]. Two lower bounds were obtained in [4] for the average genus of two kinds of graphs. In [19], Stahl gave the asymptotic result for the average genus of linear graph families. The exact values for the average genus of small-order complete graphs, closed-end ladders, and cobblestone paths were derived by White [22]. More references are the following: [5, 10, 15, 17, 20] etc. For a general background in topological graph theory, we refer the reader to see Gross and Tucker [13] or White [21].

One of the purposes of the paper is to give an explicit expression of the average genus for a bouquet of circles. By a *bouquet of circles*, or more briefly, a bouquet, we mean a graph with one vertex and some self-loops. In particular, the bouquet with n self-loops is denoted by B_n . Figure 1 shows the graphs B_1, B_2, B_3 . The bouquets $\{B_n, n \geq 1\}$ are very important graphs in topological graph theory. First, since any connected graph can be reduced to a bouquet by contracting a spanning tree to a point, bouquets are fundamental building blocks of topological graph theory. Second, as shown in [8, 12], Cayley graphs and many other regular graphs are covering spaces of bouquets.

For the genus distribution of B_n , Gross, Robbins and Tucker [11] proved that the numbers $g_k(B_n)$ of embeddings of the B_n in an oriented surface of genus k satisfy the following recurrence for $n > 2$,

$$(n + 1)g_k(B_n) = 4(2n - 1)(2n - 3)(n - 1)^2(n - 2)g_{k-1}(B_{n-2}) + 4(2n - 1)(n - 1)g_k(B_{n-1}) \tag{1.2}$$

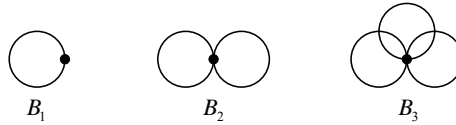


Figure 1: The bouquets $B_1, B_2,$ and B_3 .

with initial conditions

$$\begin{aligned}
 g_k(B_0) &= 1 \text{ for } k = 0 \text{ and } g_k(B_0) = 1 \text{ for } k > 0, \\
 g_k(B_1) &= 1 \text{ for } k = 0 \text{ and } g_k(B_1) = 1 \text{ for } k > 0.
 \end{aligned}
 \tag{1.3}$$

With the aid of an edge-attaching surgery technique, the total embedding polynomial of B_n was computed in [14]. Stahl [18] also did some research on the average genus of B_n . By [18, Theorem 2.5] and the definition of Euler-Mascheroni constant, one easily sees that

$$\lim_{n \rightarrow \infty} \left(\gamma_{\text{avg}}(B_n) - \left(\frac{n+1}{2} - \frac{1}{2} \sum_{k=1}^{2n} \frac{1}{k} \right) \right) = 0.
 \tag{1.4}$$

To achieve this, Stahl made many accurate estimates on the unsigned Stirling numbers $s(n, k)$ of the first kind. In this paper, using knowledge in ordinary differential equations and Taylor’s formula, we derive an explicit expression of $\gamma_{\text{avg}}(B_n)$. By this expression, (1.4) follows immediately. Our methods are totally different from that in [18] and we do not need to make estimates on $s(n, k)$. In Section 2, we will give the computation of $\gamma_{\text{avg}}(B_n)$ in detail.

A dipole with n edges, denoted by D_n , has two vertices joined by n edges. Figure 2 shows the graphs D_1, D_2, D_3 .

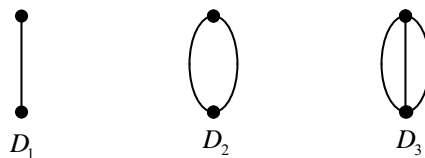


Figure 2: The dipoles $D_1, D_2,$ and D_3 .

Another purpose of this paper is to give an explicit expression of the average genus for *dipole* D_n . The dipole, like the bouquet, is useful as a voltage graph. See [21] for example. Moreover, hypermaps correspond with the 2-cell embeddings of the dipole. The genus distribution of D_n is given by [14] and [16].

In Lemma 2.1 below, we obtain the following recurrence relation for $\gamma_{\text{avg}}(B_n)$

$$(n+1)\gamma_{\text{avg}}(B_n) = 2\gamma_{\text{avg}}(B_{n-1}) + (n-1)(\gamma_{\text{avg}}(B_{n-2}) + 1).
 \tag{1.5}$$

The most popular way to deal with sequences of numbers is to manipulate infinite series that “generate” those sequences. For instance, see [6, 7]. We apply this method to

the calculation of $\gamma_{\text{avg}}(B_n)$. Multiplying both sides of (1.5) by t^n and summing on $n \geq 1$, the generating function $u(t) = \sum_{n \geq 1} \gamma_{\text{avg}}(B_n)t^n$ will satisfy an ordinary differential equation. We solve this differential equation with the aid of a computer system and find an explicit expression for $\gamma_{\text{avg}}(B_n)$ by expanding $u(t)$ as a power series in t . The calculation of $\gamma_{\text{avg}}(D_n)$ is similar to that in $\gamma_{\text{avg}}(B_n)$. But the processes are more complicated, so we still give their details in Section 3.

2 The average genus of B_n

We begin by proving the following lemma.

Lemma 2.1. *The following recurrence relation holds for the average genus $\gamma_{\text{avg}}(B_n)$ of B_n*

$$(n + 1)\gamma_{\text{avg}}(B_n) = 2\gamma_{\text{avg}}(B_{n-1}) + (n - 1)(\gamma_{\text{avg}}(B_{n-2}) + 1) \tag{2.1}$$

with initial conditions $\gamma_{\text{avg}}(B_1) = 0, \gamma_{\text{avg}}(B_2) = \frac{1}{3}$.

Proof. Multiplying both sides of (1.2) by x^k and summing on $k \geq 0$, it holds that

$$\begin{aligned} \sum_{k \geq 0} (n + 1)g_k(B_n)x^k &= \sum_{k \geq 0} 4(2n - 1)(2n - 3)(n - 1)^2(n - 2)g_{k-1}(B_{n-2})x^k \\ &\quad + \sum_{k \geq 0} 4(2n - 1)(n - 1)g_k(B_{n-1})x^k. \end{aligned} \tag{2.2}$$

Hence, the genus polynomial $\Gamma_{B_n}(x)$ satisfies the following recurrence

$$(n + 1)\Gamma_{B_n}(x) = 4(2n - 1)(2n - 3)(n - 1)^2(n - 2) \cdot x \cdot \Gamma_{B_{n-2}}(x) + 4(2n - 1)(n - 1)\Gamma_{B_{n-1}}(x). \tag{2.3}$$

Differentiating both sides of (2.3) and taking $x = 1$ lead to

$$\begin{aligned} (n + 1)\Gamma'_{B_n}(1) &= 4(2n - 1)(2n - 3)(n - 1)^2(n - 2) \cdot \Gamma'_{B_{n-2}}(1) \\ &\quad + 4(2n - 1)(2n - 3)(n - 1)^2(n - 2) \cdot \Gamma_{B_{n-2}}(1) + 4(2n - 1)(n - 1)\Gamma'_{B_{n-1}}(1). \end{aligned}$$

Applying (1.1) to the graph B_n yields $\Gamma_{B_n}(1) = (2n - 1)!$. Dividing both sides of the above equality by $\Gamma_{B_n}(1)$, by the definition of average genus, one arrives at

$$(n + 1)\gamma_{\text{avg}}(B_n) = 2\gamma_{\text{avg}}(B_{n-1}) + (n - 1)(\gamma_{\text{avg}}(B_{n-2}) + 1).$$

A direct calculation gives rise to $\gamma_{\text{avg}}(B_1) = 0$ and $\gamma_{\text{avg}}(B_2) = \frac{1}{3}$. The proof is completed. □

The main purpose of this section is to prove the following theorem.

Theorem 2.2. *The average genus of B_n is given by*

$$\gamma_{\text{avg}}(B_n) = \frac{n + 1}{2} - \sum_{m=0}^{n-1} \frac{1 + (-1)^m}{2(m + 1)} - \frac{1 + (-1)^n}{4(n + 1)}. \tag{2.4}$$

In particular, we have

$$\gamma_{\text{avg}}(B_n) = \frac{n - \ln n - \gamma + 1 - \ln 2}{2} + o(1),$$

where $\gamma \approx 0.5772$ is the Euler-Mascheroni constant.

Proof. For $n \leq 0$, we define $\gamma_{\text{avg}}(B_n) = 0$ so that (2.1) holds for any integer $n \geq 1$. For the simplicity of writing, we use a_n to denote $\gamma_{\text{avg}}(B_n)$ in the proof. Multiplying both sides of (2.1) by t^n and summing on $n \geq 1$, we obtain

$$\sum_{n \geq 1} (n+1)a_n t^n = 2 \sum_{n \geq 1} a_{n-1} t^n + \sum_{n \geq 1} (n-1)(a_{n-2} + 1)t^n. \tag{2.5}$$

Let $u(t) = \sum_{n \geq 1} a_n t^n$. Then, with the help of (2.5), we obtain

$$\begin{aligned} \left(t \cdot \sum_{n \geq 1} a_n t^n\right)' &= 2t \cdot \sum_{n \geq 1} a_{n-1} t^{n-1} + \sum_{n \geq 1} (n-2)a_{n-2} t^n + \sum_{n \geq 1} a_{n-2} t^n + \sum_{n \geq 1} (n-1)t^n \\ &= 2tu(t) + t^3 \sum_{n \geq 1} (n-2)a_{n-2} t^{n-3} + t^2 u(t) + t^2 \cdot \left(\sum_{n \geq 2} t^{n-1}\right)', \end{aligned}$$

that is

$$\begin{aligned} (tu(t))' &= 2tu(t) + t^3 \sum_{n \geq 3} (n-2)a_{n-2} t^{n-3} + t^2 u(t) + t^2 \left(\frac{t}{1-t}\right)' \\ &= 2tu(t) + t^3 \sum_{n \geq 1} n a_n t^{n-1} + t^2 u(t) + t^2 \left(\frac{t}{1-t}\right)' \\ &= 2tu(t) + t^3 u'(t) + t^2 u(t) + t^2 \left(\frac{t}{1-t}\right)', \end{aligned}$$

which implies that $u(t)$ satisfies the following equation

$$(t - t^3)u'(t) + (1 - 2t - t^2)u(t) = \frac{t^2}{(1-t)^2} \tag{2.6}$$

with initial condition $u(0) = 0$. Since the above equation is a first order linear differential equation, we can solve it directly and obtain its solution:

$$u(t) = \frac{-(t^2 - 1) \ln(1-t) + (t^2 - 1) \ln(t+1) + 2t}{4(t-1)^2 t}.$$

Denote

$$u_1(t) = \frac{1}{2(t-1)^2}, \quad u_2(t) = -\frac{(t+1) \ln(1-t)}{4(t-1)t}, \quad u_3(t) = \frac{(t+1) \ln(t+1)}{4(t-1)t}.$$

Then, clearly, $u(t) = u_1(t) + u_2(t) + u_3(t)$. Using Taylor's formula, we get

$$u_1(t) = \sum_{n \geq 0} \frac{n+1}{2} t^n \tag{2.7}$$

and

$$u_2(t) = \frac{1}{4}(1+t) \cdot \frac{1}{1-t} \cdot \frac{\ln(1-t)}{t} = \frac{1}{4}(1+t) \cdot \sum_{\ell \geq 0} t^\ell \cdot \sum_{m \geq 0} \left(-\frac{1}{m+1} t^m\right)$$

$$= \frac{1}{4}(1+t) \cdot \sum_{n \geq 0} \sum_{m=0}^n \left(-\frac{1}{m+1}\right) t^n = \sum_{n \geq 0} b_n t^n, \tag{2.8}$$

where $b_0 = -\frac{1}{4}$ and $b_n = \frac{1}{4} \left[\sum_{m=0}^n \left(-\frac{1}{m+1}\right) + \sum_{m=0}^{n-1} \left(-\frac{1}{m+1}\right) \right], n \geq 1$. Also by the Taylor’s formula,

$$\begin{aligned} u_3(t) &= -\frac{1}{4}(1+t) \cdot \frac{1}{1-t} \cdot \frac{\ln(1+t)}{t} = -\frac{1}{4}(1+t) \cdot \sum_{\ell \geq 0} t^\ell \cdot \sum_{m \geq 0} \frac{(-1)^m}{m+1} t^m \\ &= -\frac{1}{4}(1+t) \cdot \sum_{n \geq 0} \sum_{m=0}^n \frac{(-1)^m}{m+1} t^n = \sum_{n \geq 0} c_n t^n, \end{aligned} \tag{2.9}$$

where $c_0 = -\frac{1}{4}$ and

$$c_n = -\frac{1}{4} \left[\sum_{m=0}^n \frac{(-1)^m}{m+1} + \sum_{m=0}^{n-1} \frac{(-1)^m}{m+1} \right], \quad n \geq 1.$$

It follows from (2.7)–(2.9) that

$$\begin{aligned} a_n &= \frac{n+1}{2} + b_n + c_n = \frac{n+1}{2} + \frac{1}{4} \left[\sum_{m=0}^n \left(-\frac{1}{m+1}\right) + \sum_{m=0}^{n-1} \left(-\frac{1}{m+1}\right) \right] \\ &\quad - \frac{1}{4} \left[\sum_{m=0}^n \frac{(-1)^m}{m+1} + \sum_{m=0}^{n-1} \frac{(-1)^m}{m+1} \right], \end{aligned}$$

which yields (2.4). In view of

$$\gamma = \lim_{n \rightarrow +\infty} \left[\sum_{m=0}^n \frac{1}{m+1} - \ln n \right] \quad \text{and} \quad \lim_{n \rightarrow +\infty} \sum_{m=0}^{n-1} \frac{(-1)^m}{m+1} = \ln 2, \tag{2.10}$$

we complete the proof of (2.2). □

3 The average genus of D_n

Our first purpose is to show the following lemma.

Lemma 3.1. *The following recurrence relation holds for the average genus $\gamma_{\text{avg}}(D_n)$ of D_n*

$$n(n+2)\gamma_{\text{avg}}(D_{n+1}) = (2n+1)\gamma_{\text{avg}}(D_n) + (n^2-1) \cdot \gamma_{\text{avg}}(D_{n-1}) + n^2 \tag{3.1}$$

with initial conditions $\gamma_{\text{avg}}(D_1) = \gamma_{\text{avg}}(D_2) = 0$.

Proof. By [16, Theorem 5.2], we obtain

$$(n+2)g_k(D_{n+1}) = n(2n+1)g_k(D_n) + n^3(n-1)^2g_{k-1}(D_{n-1}) - n(n-1)^2g_k(D_{n-1}).$$

Applying (1.1) to the graph D_{n+1} yields $\Gamma_{D_{n+1}}(1) = (n!)^2$. Following the lines in the proof of Lemma 2.1, we derive the recurrence relation (3.1).

The initial conditions $\gamma_{\text{avg}}(D_1) = \gamma_{\text{avg}}(D_2) = 0$ are due to a direct calculation. The proof is finished. □

The main purpose of this section is to prove the following theorem.

Theorem 3.2. $\gamma_{\text{avg}}(D_1) = \gamma_{\text{avg}}(D_2) = 0$ and for $n \geq 3$, we have

$$\begin{aligned} \gamma_{\text{avg}}(D_n) = n \left[\frac{1}{2} \sum_{m=4}^{n+1} \frac{(-1)^m(4m^2 - 12m + 6)}{(m-3)(m-2)(m-1)m} + \frac{1}{6} \right] - \frac{1}{2} \sum_{m=1}^{n+1} \frac{1}{m} \\ - \sum_{m=4}^{n+1} \frac{(-1)^m(2m^2 - 6m + 3)}{(m-3)(m-1)m} + \frac{7}{12}. \end{aligned} \tag{3.2}$$

In particular, we have

$$\gamma_{\text{avg}}(D_n) = \frac{n - \ln n - \gamma}{2} + o(1), \tag{3.3}$$

where $\gamma \approx 0.5772$ is the Euler-Mascheroni constant.

Proof. First, we give a proof of (3.2). For the simplicity of writing, we use a_n to denote $\gamma_{\text{avg}}(D_n)$ in the proof. Let $u(t) = \sum_{n \geq 1} a_n t^{n-3} = \sum_{n \geq 2} a_{n+1} t^{n-2}$. Multiplying both sides of (3.1) by t^{n-2} and summing on $n \geq 2$, we obtain

$$\begin{aligned} \sum_{n \geq 2} n(n+2)a_{n+1}t^{n-2} = \sum_{n \geq 2} (2n+1)a_n t^{n-2} \\ + \sum_{n \geq 2} (n^2-1)a_{n-1}t^{n-2} + \sum_{n \geq 2} n^2 t^{n-2}. \end{aligned} \tag{3.4}$$

Since

$$\begin{aligned} u'(t) &= \sum_{n \geq 2} (n-2)a_{n+1}t^{n-3}, \\ u''(t) &= \sum_{n \geq 2} (n-2)(n-3)a_{n+1}t^{n-4}, \end{aligned}$$

it follows that

$$\begin{aligned} \sum_{n \geq 2} n(n+2)a_{n+1}t^{n-2} &= \sum_{n \geq 2} [(n-2)(n-3) + 7(n-2) + 8]a_{n+1}t^{n-2} \\ &= t^2u''(t) + 7tu'(t) + 8u(t), \\ \sum_{n \geq 2} (2n+1)a_n t^{n-2} &= \sum_{n \geq 2} (2n+3)a_{n+1}t^{n-1} = \sum_{n \geq 2} (2(n-2) + 7)a_{n+1}t^{n-1} \\ &= 2t^2u'(t) + 7tu(t), \\ \sum_{n \geq 2} (n^2-1)a_{n-1}t^{n-2} &= \sum_{n \geq 4} (n^2-1)a_{n-1}t^{n-2} = \sum_{n \geq 2} (n^2 + 4n + 3)a_{n+1}t^n \\ &= \sum_{n \geq 2} [(n-2)(n-3) + 9(n-2) + 15]a_{n+1}t^n \\ &= t^4u''(t) + 9t^3u'(t) + 15t^2u(t), \\ \sum_{n \geq 2} n^2t^{n-2} &= \sum_{n \geq 2} n(n-1)t^{n-2} + \sum_{n \geq 2} nt^{n-2} = v''(t) + \sum_{n \geq 0} nt^{n-2} - t^{-1} \\ &= v''(t) + \frac{v'(t)}{t} - t^{-1} = \frac{3t-4-t^2}{(t-1)^3}, \end{aligned}$$

where $v(t) = \sum_{n \geq 0} t^n$, $v'(t) = \sum_{n \geq 0} nt^{n-1}$, $v''(t) = \sum_{n \geq 0} n(n-1)t^{n-2}$. Substituting the above equalities into (3.4), $u(t)$ satisfies the following second order linear differential equation

$$(t^2 - t^4)u''(t) + (7t - 2t^2 - 9t^3)u'(t) + (8 - 7t - 15t^2)u(t) = \frac{3t - 4 - t^2}{(t - 1)^3}$$

with initial conditions $u(0) = a_3 = \gamma_{\text{avg}}(D_3) = \frac{1}{2}$, $u'(0) = a_4 = \gamma_{\text{avg}}(D_4) = \frac{5}{6}$.

With the help of a computer algebra systems, the solution of the above equation is

$$u(t) = \frac{1}{4(t - 1)t^2} + \frac{w(t)}{4(t - 1)^2t^4}, \tag{3.5}$$

where

$$w(t) = -t^3 + 2t^3 \ln(t + 1) + 3t^2 - 2t^2 \ln(t + 1) - 2t \ln(1 - t) - 2t \ln(t + 1) + 2 \ln(1 - t) + 2 \ln(t + 1).$$

By Taylor’s formula, we get

$$\begin{aligned} \frac{1}{4(t - 1)t^2} &= \sum_{m \geq -2} \left(-\frac{1}{4}\right)t^m, \\ w(t) &= t^2 - t^3 \\ &\quad + \sum_{m \geq 4} \frac{2(4(-1)^m m^2 + m^2 - 12(-1)^m m - 5m + 6(-1)^m + 6)}{(m - 3)(m - 2)(m - 1)m} t^m, \\ \frac{1}{4(t - 1)^2t^4} &= \sum_{m \geq -4} \frac{m + 5}{4} t^m. \end{aligned}$$

Therefore, comparing the coefficients of t^{n-3} of the both sides of (3.5) gives

$$\begin{aligned} a_n &= -\frac{1}{4} + \frac{n}{4} - \frac{n - 1}{4} \\ &\quad + \sum_{m=4}^{n+1} \frac{2(4(-1)^m m^2 + m^2 - 12(-1)^m m - 5m + 6(-1)^m + 6)}{(m - 3)(m - 2)(m - 1)m} \cdot \frac{n - m + 2}{4} \\ &= \frac{n}{2} \sum_{m=4}^{n+1} \left[\frac{(-1)^m (4m^2 - 12m + 6)}{(m - 3)(m - 2)(m - 1)m} + \frac{(m^2 - 5m + 6)}{(m - 3)(m - 2)(m - 1)m} \right] \\ &\quad - \sum_{m=4}^{n+1} \frac{(-1)^m (4m^2 - 12m + 6) + (m^2 - 3m) + (-2m + 6)}{(m - 3)(m - 2)(m - 1)m} \cdot \frac{m - 2}{2} \\ &= \frac{n}{2} \sum_{m=4}^{n+1} \frac{(-1)^m (4m^2 - 12m + 6)}{(m - 3)(m - 2)(m - 1)m} + \frac{n}{2} \sum_{m=4}^{n+1} \frac{1}{(m - 1)m} \\ &\quad - \frac{1}{2} \sum_{m=4}^{n+1} \frac{(-1)^m (4m^2 - 12m + 6)}{(m - 3)(m - 1)m} - \frac{1}{2} \sum_{m=4}^{n+1} \frac{1}{m - 1} + \sum_{m=4}^{n+1} \frac{1}{m(m - 1)} \end{aligned}$$

$$\begin{aligned}
 &= \frac{n}{2} \sum_{m=4}^{n+1} \frac{(-1)^m(4m^2 - 12m + 6)}{(m - 3)(m - 2)(m - 1)m} + \frac{n}{2} \left(\frac{1}{3} - \frac{1}{n + 1} \right) \\
 &\quad - \frac{1}{2} \sum_{m=4}^{n+1} \frac{(-1)^m(4m^2 - 12m + 6)}{(m - 3)(m - 1)m} - \frac{1}{2} \sum_{m=1}^{n+1} \frac{1}{m} \\
 &\quad + \frac{3}{4} + \frac{1}{2(n + 1)} + \left(\frac{1}{3} - \frac{1}{n + 1} \right)
 \end{aligned}$$

which yields the desired result (3.2).

Now we are in a position to prove (3.3). Using the software *Mathematica* or series theory, one has

$$\sum_{m=4}^{n+1} \frac{(-1)^m(4m^2 - 12m + 6)}{(m - 3)(m - 2)(m - 1)m} = \frac{2}{3} + o\left(\frac{1}{n}\right) \tag{3.6}$$

and

$$\sum_{m=4}^{n+1} \frac{(-1)^m(2m^2 - 6m + 3)}{(m - 3)(m - 1)m} = \frac{7}{12} + o(1). \tag{3.7}$$

Combining (3.6)–(3.7), (2.10) and (3.2), we complete the proof of (3.3). □

4 Some remarks

Bouquets and dipoles are two important classes of graphs in topological graph theory. Their average genera are of independent interest. In this paper, we obtain explicit formulas for $\gamma_{\text{avg}}(B_n)$ and $\gamma_{\text{avg}}(D_n)$. By Theorems 2.2 and 3.2, we have the following relation between $\gamma_{\text{avg}}(B_n)$ and $\gamma_{\text{avg}}(D_n)$,

$$\gamma_{\text{avg}}(B_n) = \gamma_{\text{avg}}(D_n) + \frac{1 - \ln 2}{2} + o(1).$$


It follows that the difference of $\gamma_{\text{avg}}(B_n)$ and $\gamma_{\text{avg}}(D_n)$ tends to the constant $\frac{1 - \ln 2}{2}$ when n tends to infinity.

Since both B_n and D_n are upper-embeddable, the maximum genera of B_n and D_n are $\lfloor \frac{n}{2} \rfloor$ and $\lfloor \frac{n-1}{2} \rfloor$, respectively. Recall that the minimum genera of B_n and D_n equal 0. Therefore, also by Theorems 2.2 and 3.2, we have

$$\lim_{n \rightarrow \infty} \frac{\gamma_{\text{avg}}(B_n)}{\lfloor \frac{n}{2} \rfloor} = 1 \text{ and } \lim_{n \rightarrow \infty} \frac{\gamma_{\text{avg}}(D_n)}{\lfloor \frac{n-1}{2} \rfloor} = 1.$$

This implies that the average genus of B_n (D_n) is closer to the maximum genus than to the minimum genus.

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Well-totally-dominated graphs*

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Abstract

A subset of vertices in a graph is called a total dominating set if every vertex of the graph is adjacent to at least one vertex of this set. A total dominating set is called minimal if it does not properly contain another total dominating set. In this paper, we study graphs whose all minimal total dominating sets have the same size, referred to as well-totally-dominated (WTD) graphs. We first show that WTD graphs with bounded total domination number can be recognized in polynomial time. Then we focus on WTD graphs with total domination number two. In this case, we characterize triangle-free WTD graphs and WTD graphs with packing number two, and we show that there are only finitely many planar WTD graphs with minimum degree at least three. Lastly, we show that if the minimum degree is at least three then the girth of a WTD graph is at most 12. We conclude with several open questions.

Keywords: Total domination, well-totally-dominated graphs, minimal total dominating sets.

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1 Introduction

Total domination in graphs has been extensively studied in the literature (see [15]) and has numerous applications. For instance, consider a computer network where a core group of file servers has the ability to communicate directly with every computer outside the core group. Moreover, each file server is directly linked to at least one other backup file server where duplicate information is stored. This core group of servers corresponds to a total dominating set in the graph representing the computer network. Another application area is a specific committee selection mechanism such that every non-member of the committee knows at least one member of the committee and every member of the committee knows at least one other member of the committee to avoid feelings of isolation and thus enhance cooperation (see [14]).

Let G be a graph with no isolated vertices. A subset S of $V(G)$ is called a *total dominating set* (TDS) of G if every vertex in G is adjacent to at least one element in S . A total dominating set is *minimal* if it contains no other TDS of G . The minimum size of a total dominating set of a graph G is called the *total domination number* and denoted by $\gamma_t(G)$, while the maximum size of a minimal total dominating set is called the *upper total domination number* and denoted by $\Gamma_t(G)$. G is called *well-totally-dominated* (WTD) if every minimal TDS of G is of the same size, that is, $\gamma_t(G) = \Gamma_t(G)$. WTD graphs with $\gamma_t = k$ are denoted by $\text{WTD}(k)$.

Given a graph, computing its total domination number and its upper total domination number are NP-hard in general [6, 18] and already NP-hard even in specific graph classes such as bipartite graphs, comparability graphs and claw-free graphs [15]. One way to deal with such a problem is to consider “trivial” instances where these two parameters have the same value. Examples of graph classes defined in this way in the literature include well-covered graphs (whose all maximal independent sets have the same size), well-dominated graphs (whose all minimal dominating sets have the same size), and equimatchable graphs (whose all maximal matchings have the same size). Structural properties of each one of these graph classes have been studied extensively in the literature. In this paper, we take the same approach for the total dominating sets. Works on total domination in the literature mostly focused on the relation of the total domination number with other graph parameters and characterized graphs with total domination number being equal to an upper bound (e.g. [3, 4]). Inequalities relating the total domination number to other domination parameters and characterization of graphs that tightly attain these bounds have also been studied (see [1, 16]).

Clearly, if the total domination number and the upper total domination number are polynomial time solvable for a given class of graphs, then the recognition of WTD graphs belonging to this class of graphs is polynomial. However, the complexity of recognizing WTD graphs in general is unknown. In such a situation, a classical approach consists in studying the structure of WTD graphs in restricted graph classes and providing structural characterizations along with efficient recognition algorithms whenever possible.

WTD graphs were initially introduced in [12], where WTD cycles and paths are characterized and several constructions of WTD trees are given. They also proved that a WTD graph with minimum degree at least two has girth at most 14. The work in [7] focused on the composition and decomposition of WTD trees and proved that any WTD tree can be constructed from a family of three small trees. To the best of our knowledge, [12] and [7] are the only work on WTD graphs. A graph class resembling WTD graphs is *well-dominated graphs*, which are graphs whose minimal dominating sets have the same size. It

is known that well-dominated graphs form a proper subset of well-covered graphs [8]. We note that well-covered graphs are graphs whose maximal independent sets have the same size and there is a rich literature about them (see [13, 19]). Well-dominated graphs were introduced by Finbow et al. [8], who provided a characterization of bipartite well-dominated graphs and well-dominated graphs with girth at least 5. Characterizations of these graphs within other graph classes were also obtained [9, 10, 17, 20]. Although their definitions resemble each other, there is not a containment relationship between WTD graphs and well-dominated graphs. For instance, a cycle on six vertices is WTD but not well-dominated, whereas the graph T_{10} described in [17] is well-dominated but not WTD.

It follows from the previous studies on WTD graphs that we do not know much about their structure. In this paper, we investigate the study of WTD graphs from a structural point of view. We first study WTD graphs with bounded total domination number. We prove in Section 2 that the recognition of WTD graphs with total domination number k is solvable in polynomial time for every positive integer k . We then focus on WTD graphs with total domination number 2, referred to as WTD(2) graphs in Section 3. We characterize triangle-free WTD(2) graphs and WTD(2) graphs with packing number 2 (or equivalently of diameter 3). We also show that there is a finite number of planar WTD(2) graphs with minimum degree at least 3. Subsequently, we study the girth of WTD graphs in Section 4. In particular, building on a result in [12], we prove that WTD graphs with minimum degree at least three have girth at most 12. Finally, we discuss several open research directions.

2 WTD graphs with bounded total domination number

Recall that the complexity of recognizing WTD graphs is unknown. In this section, we show that for any positive integer k , WTD(k) graphs can be recognized in polynomial time. To this end, we will use an equivalent description of WTD(k) graphs using transversal hypergraphs. Let us first introduce necessary definitions. A *hypergraph* H is a pair $H = (X, E)$ where X is a set of elements called *vertices*, and E is a set of nonempty subsets of X called *hyperedges*. Therefore, a hypergraph might have a vertex which belongs to none of the hyperedges, but cannot have multiple hyperedges. A *transversal* (or *hitting set*) of a hypergraph $H = (X, E)$ is a set $T \subseteq X$ that has nonempty intersection with every hyperedge of H . A transversal of a collection of sets is a transversal of the hypergraph whose hyperedges are the given collection. A transversal T is called *minimal* if no proper subset of T is a transversal. The *transversal hypergraph* of $H = (X, E)$ is the hypergraph $H^* = (X, F)$ whose hyperedge set F consists of all minimal transversals of H .

Let G be a graph with no isolated vertex. Let H_G be the hypergraph whose vertex set is $V(G)$ and hyperedges are open neighborhoods of the vertices of G . Let also $\text{MTDS}(G)$ denote the set of all minimal total dominating sets of G .

Lemma 2.1. *MTDS(G) consists of hyperedges of the transversal hypergraph of H_G .*

Proof. Let T be a hyperedge of H_G^* , that is a minimal transversal of the set of open neighborhoods of G . This means that T contains a neighbor of every vertex in G , thus it is a total dominating set. By minimality of the transversal T , it is also a minimal total dominating set of G . Conversely, let S be a minimal total dominating set of G . Then, every vertex in G is adjacent to at least one vertex in S . That is, S has a nonempty intersection with every open neighborhood in G . Therefore, S is a transversal of the hypergraph H_G and minimality of S implies that it is a minimal transversal. Thus, S is a hyperedge of H_G^* . \square

Proposition 2.2. *Let G be a graph. Then, for any minimal transversal T of $\text{MTDS}(G)$, there exists a vertex v in G such that $N(v) = T$.*

Proof. Let $\text{MTDS}(G) = \{A_1, \dots, A_m\}$. Since T has nonempty intersection with each A_i , $V(G) \setminus T$ contains none of the minimal total dominating sets A_1, \dots, A_m . Therefore, $V(G) \setminus T$ is not a TDS of G , and hence there exists at least one vertex $v \in V(G)$ such that $N(v) \cap (V(G) \setminus T) = \emptyset$. Thus, we see that $N(v) \subseteq T$. Suppose that $N(v) \neq T$. Then $T \setminus N(v) \neq \emptyset$ and let $u \in T \setminus N(v)$. Since T is a minimal transversal, $T \setminus \{u\}$ is disjoint with at least one of A_1, \dots, A_m , say A_1 . As $u \in T \setminus N(v)$, we have $N(v) \subseteq T \setminus \{u\}$, and hence $N(v) \cap A_1 = \emptyset$. That is, v is not dominated by A_1 , which is a contradiction. Therefore, $N(v) = T$. \square

A hypergraph H is said to be *Sperner* if no hyperedge of H contains another hyperedge. The following result shows that any finite collection of finite sets which forms a Sperner hypergraph corresponds to the set of all minimal total dominating sets of a graph.

Proposition 2.3. *Let H be a Sperner hypergraph. Then there exists a graph G such that $E(H) = \text{MTDS}(G)$.*

Proof. Let $E(H) = \{A_1, \dots, A_m\}$ and $A = \cup_{i=1}^m A_i$. Consider a graph with vertex set A and draw edges between its vertices such that each vertex is adjacent to at least one vertex in A_i for all $i = 1, \dots, m$ (for example, draw all possible edges). Then, in accordance with Proposition 2.2, for each minimal transversal T of H , add a vertex v_T to the graph such that $N(v_T) = T$. Let G be the resulting graph.

We first show that each A_i is a TDS of G . By construction, every vertex of A is adjacent to at least one vertex in A_i . Moreover, for every minimal transversal T of A_1, \dots, A_m we have $T \cap A_i \neq \emptyset$, and hence, each v_T is dominated by A_i . Therefore, A_i is a TDS for $i = 1, \dots, m$.

We next show that every TDS of G contains at least one of A_1, \dots, A_m . Let S be a TDS of G and suppose that $A_i \not\subseteq S$ for $i = 1, \dots, m$. Then, $V(G) \setminus S$ is a transversal of A_1, \dots, A_m , and hence, there exists a minimal transversal T of A_1, \dots, A_m such that $T \subseteq V(G) \setminus S$. On the other hand, we have $N(v_T) = T$ and thus, we get $N(v_T) \cap S = \emptyset$, which contradicts that S is a TDS of G .

Consequently, a set other than A_1, \dots, A_m can not be a minimal TDS of G . We finally show that each A_i is a minimal TDS of G . Suppose that A_i is not minimal for some i . Then, $A_i \setminus \{x\}$ is still a TDS of G for some $x \in A_i$, and therefore, $A_j \subseteq A_i \setminus \{x\}$ for some j , which implies $A_j \subseteq A_i$ contradicting that H is Sperner. Therefore, minimal TDSs of G are exactly A_1, \dots, A_m . \square

Remark 2.4. One can extend G to another graph whose minimal TDSs are A_1, \dots, A_m as follows: Let G' be a graph disjoint from G . Draw edges between the vertices of G' and A in such a way that every vertex of G' is adjacent to at least one vertex of A_i for $i = 1, \dots, m$. By following the same arguments, it is easy to check that minimal TDSs of the resulting graph are A_1, \dots, A_m .

Notice that any finite collection consisting of distinct sets of size k corresponds to a Sperner hypergraph and therefore, Proposition 2.3 implies the following result.

Corollary 2.5. *For every integer $k \geq 2$, $\text{WTD}(k)$ is an infinite graph family.*

The HYPERGRAPH TRANSVERSAL problem is the decision problem that takes as input two Sperner hypergraphs H and H' and asks whether H' is the transversal hypergraph H^* of H .

Theorem 2.6 ([2, 5]). *For every positive integer k , the HYPERGRAPH TRANSVERSAL problem is solvable in polynomial time if all hyperedges of one of the two hypergraphs H and H' are of size at most k .*

Theorem 2.6 has the following consequence:

Corollary 2.7 ([11]). *For every positive integer k , the following problem is solvable in polynomial time: Given a Sperner hypergraph H , determine whether all minimal transversals of H are of size k .*

The complexity of recognition of WTD graphs with bounded total domination number can now be derived from Corollary 2.7.

Theorem 2.8. *For every positive integer k , the problem of recognizing $WTD(k)$ graphs can be solved in polynomial time.*

Proof. Let G be a graph with no isolated vertices. Consider the hypergraph $H_G = (V, \mathcal{E})$, where \mathcal{E} contains the inclusion-minimal elements of $\{N(v) : v \in V\}$. Observe that H_G is Sperner and that the minimal transversals of H_G are exactly the minimal total dominating sets of G by Lemma 2.1. It follows that G is WTD if and only if all minimal transversals of H_G are of size k . By Corollary 2.7, this condition can be tested in polynomial time. \square

3 WTD graphs with total domination number two

In this section, we study WTD graphs whose total domination number is 2. We give complete characterizations of $WTD(2)$ graphs with packing number 2 and triangle-free $WTD(2)$ graphs. We also show that planar $WTD(2)$ graphs with minimum degree at least 3 have at most 16 vertices.

Let G be a $WTD(2)$ graph. Note that every minimal TDS of G is a pair consisting of endpoints of an edge of G . Consequently, every $WTD(2)$ graph is connected. We will call an edge of G whose endpoints is a TDS of G a *dominating edge* of G . Let G_{de} be the graph with vertex set $\cup_{S \in \text{MTDS}(G)} S$ (i.e., vertices of G serve as an endpoint of a dominating edge) and edge set which consists of dominating edges of G . In other words, G_{de} is the edge-induced subgraph of G obtained by the dominating edges. See Figure 1 for an example.

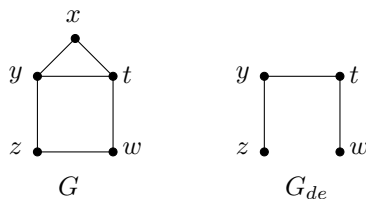


Figure 1: A $WTD(2)$ graph G and the graph G_{de} obtained by the dominating edges of G .

Remark 3.1. Notice that the graph G_{de} and the subgraph of G induced by $V(G_{de})$ are not necessarily the same. In general, G_{de} is a subgraph of G but not necessarily an induced subgraph of G with respect to a set of vertices.

A set S is a *vertex cover* of a graph G if every edge of G has an endpoint from S . Let $MVC(G)$ denote the set of all minimal vertex covers of the graph G .

Proposition 3.2. *Let G be a WTD(2) graph. For every minimal vertex cover S of G_{de} there exists a vertex v_S in G such that $N(v_S) = S$.*

Proof. We notice that every minimal vertex cover S of G_{de} is a minimal transversal of $MTDS(G)$. Therefore, by Proposition 2.2 there exists a vertex in G whose neighborhood is exactly S . □

3.1 Characterization of WTD(2) graphs with packing number 2

A set $S \subseteq V(G)$ is called a *packing* of G if $N[u] \cap N[v] = \emptyset$ for every distinct $u, v \in S$. The *packing number* $\rho(G)$ is the maximum size of a packing of G . It is well-known that for any graph G we have $\rho(G) \leq \gamma(G) \leq \gamma_t(G)$. Therefore, if $\gamma_t(G) = 2$, then $\rho(G)$ is either 1 or 2. In this subsection, we provide a characterization of WTD(2) graphs G with $\rho(G) = 2$. In particular, this characterization allows us to construct any WTD(2) graph with $\rho(G) = 2$.

Let W_2 be the set of graphs obtained as follows:

- Step 1:** Choose a bipartite graph H with no isolated vertices.
- Step 2:** For every $S \in MVC(H)$, choose a new vertex v_S and draw edges from v_S to every vertex in S .
- Step 3:** For each edge uv in H and every $w \in V(H) \setminus \{u, v\}$, add the edges wu and/or wv if needed to make sure w is adjacent to at least one of u and v .
- Step 4:** Choose a new graph H' (might be the empty graph) which is disjoint from the current graph. Then for each edge uv in H and every $w \in V(H')$, draw at least one of the edges wu and wv .

A graph in W_2 is given in Figure 2.

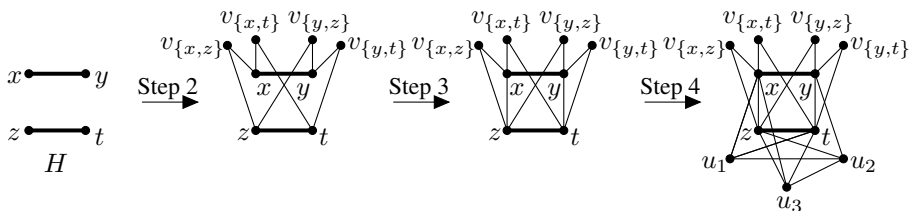


Figure 2: A graph in W_2 obtained by the given process. Bold edges represent the dominating edges.

Lemma 3.3. *If a graph G is in W_2 , then G is a WTD(2) graph with $\rho(G) = 2$.*

Proof. Let $G \in W_2$ and $H = (U, V, E)$ be the bipartite graph in the first step of the construction of G . We first show that the packing number of G is 2. As H has no isolated vertices, both U and V are minimal vertex covers of H . Thus, the vertices v_U and v_V have disjoint closed neighborhoods since $N(v_U) = U$ and $N(v_V) = V$ and hence, we get $\rho(G) \geq 2$. Clearly, by construction, every edge of H is a dominating edge of G . Therefore, we get $\gamma_t(G) = 2$. Since $\rho(G) \leq \gamma_t(G)$, we obtain $\rho(G) \leq 2$ and hence, $\rho(G) = 2$.

Now let T be a minimal TDS of G other than the edges of H . Then T contains at most one endpoint of an edge of H because otherwise T contains a TDS, which contradicts that T is minimal. Therefore, $V(H) \setminus T$ is a vertex cover of H and hence, it contains a minimal vertex cover S of H . By construction there exists a vertex v_S with $N(v_S) = S$. As $S \subseteq V(H) \setminus T$, we obtain $N(v_S) \cap T = \emptyset$, which contradicts that T is a TDS of G . Consequently, edges of H are the only minimal TDSs of G and hence, G is a WTD(2) graph and $G_{de} = H$. \square

Lemma 3.4. *Let G be a WTD(2) graph with $\rho(G) = 2$. Then, G is in W_2 .*

Proof. Let $\{x, y\}$ be a packing with minimum $|N[x]| + |N[y]|$. Note that every dominating edge of G has one endpoint from $N(x)$ and one from $N(y)$ and hence, G_{de} is a bipartite graph, say with parts X and Y where $X \subseteq N(x)$ and $Y \subseteq N(y)$.

We next show that $X = N(x)$ and $Y = N(y)$. By symmetry, it suffices to prove $X = N(x)$. Notice that G_{de} has no isolated vertices and therefore, X is a minimal vertex cover of G_{de} . By Proposition 3.2 there exists a vertex v_X satisfying $N(v_X) = X$. Suppose that $X \neq N(x)$. Then, we get $X \subset N(x)$. Clearly $v_X \neq y$. Moreover, $v_X \notin N(y)$ since $y \notin X = N(v_X)$. Thus, we get $N[v_X] \cap N[y] = \emptyset$ and hence $\{v_X, y\}$ is a packing of G . However, we obtain $|N[v_X]| + |N[y]| < |N[x]| + |N[y]|$ since $X \subset N(x)$, which contradicts the definition of the packing $\{x, y\}$. Consequently, we get $X = N(x)$ and hence, we may take $v_X = x$. Similarly, we have $Y = N(y)$ and we may assume $v_Y = y$.

Now let S be a minimal vertex cover of G_{de} . By Proposition 3.2 there exists a vertex v_S satisfying $N(v_S) = S$. If $S = X$ or $S = Y$, we can take v_S to be x or y , respectively, and in both cases, we have $v_S \notin V(G_{de})$. Otherwise, suppose that $v_S \in V(G_{de}) = X \cup Y$. Without loss of generality, let $v_S \in X$. Then, as $X = N(x)$, we get $x \in N(v_S) = S \subseteq N(x) \cup N(y)$, which is a contradiction. Therefore, v_S is not a vertex of G_{de} , that is, $v_S \in V(G) \setminus V(G_{de})$.

Finally, we see that one can obtain the graph G by following the procedure in the definition of W_2 with the initial bipartite graph $H = G_{de}$. \square

Combining the results in Lemma 3.3 and Lemma 3.4 gives the following structural characterization of WTD(2) graphs with $\rho(G) = 2$. Moreover, by definition of the class W_2 , this provides us with a procedure to construct any WTD(2) graph with $\rho(G) = 2$.

Theorem 3.5. *A graph G is WTD(2) with $\rho(G) = 2$ if and only if $G \in W_2$.*

Given a graph G , the *diameter* of G , denoted by $\text{diam}(G)$ is the maximum length of a shortest path between any pair of vertices of G . Let G be a graph such that $\gamma_t(G) = 2$. Then, it is easy to see that $\text{diam}(G) \leq 3$. Moreover, whenever $\gamma_t(G) = 2$, we have $\text{diam}(G) = 3$ if and only if $\rho(G) = 2$ and therefore, in all the statements in Lemma 3.3, Lemma 3.4 and Theorem 3.5, the condition $\rho(G) = 2$ can be replaced with $\text{diam}(G) = 3$.

Corollary 3.6. *A graph G is WTD(2) with $\text{diam}(G) = 3$ if and only if $G \in W_2$.*

One may attempt to modify the description of W_2 graphs in order to describe all WTD(2) graphs with $\rho(G) = 1$. In the first step of the process of building a graph in W_2 , if one starts with a non-bipartite graph H with no isolated vertices, then the resulting graph is still WTD(2) but has packing number 1. However, not every WTD(2) graph G with $\rho(G) = 1$ can be obtained in this way. For example, consider the graph presented in Figure 1. To obtain this graph G , in Step 1 one should definitely choose H to be the graph with vertex set $\{z, y, t, w\}$ and edge set $\{zy, yt, tw\}$ which is indeed G_{de} . However, in Step 2 if one chooses a new vertex v_S for $S = \{y, w\}$ (which is a minimal vertex cover of G_{de}), then the graph G can not be obtained. So, the complete characterization of WTD(2) graphs with $\rho(G) = 1$ is left as an open question.

3.2 Triangle-free WTD(2) graphs

In this subsection, we provide characterization of triangle-free WTD(2) graphs.

Lemma 3.7. *If G is a triangle-free graph with $\gamma_t(G) = 2$, then G is a bipartite graph and we have*

$$\rho(G) = \begin{cases} 1, & \text{if } G \text{ is complete bipartite;} \\ 2, & \text{otherwise.} \end{cases}$$

Proof. Let uv be a dominating edge of G . Then we have $N(u) \cup N(v) = V(G)$. As G is triangle-free, none of two adjacent vertices have a common neighbor. Therefore, we have $N(u) \cap N(v) = \emptyset$ and also see that both $N(u)$ and $N(v)$ are independent sets. We consequently obtain that G is a bipartite graph with parts $N(u)$ and $N(v)$. Since $\rho(G) \leq \gamma_t(G) = 2$, we have $\rho(G) \in \{1, 2\}$. Moreover, it is clear that $\rho(G) = 1$ if and only if each vertex in $N(u)$ is adjacent to all the vertices in $N(v)$, i.e., G is a complete bipartite graph. □

For a bipartite graph with parts X and Y , define $X_u = \{x \in X : N(x) = Y\}$ and $Y_u = \{y \in Y : N(y) = X\}$. In other words, X_u (resp. Y_u) is the set of vertices in X (resp. Y) which are adjacent to every vertex in Y (resp. X). The following result characterizes all triangle-free WTD(2) graphs.

Theorem 3.8. *The following three statements are equivalent:*

- (i) G is a triangle-free WTD(2) graph.
- (ii) G is a bipartite WTD(2) graph.
- (iii) G is complete bipartite graph or G is a bipartite graph with parts X and Y such that there exist vertices $a \in X \setminus X_u$ and $b \in Y \setminus Y_u$ satisfying $N(a) = Y_u \neq \emptyset$ and $N(b) = X_u \neq \emptyset$.

Proof. By Lemma 3.7 we see that (i) implies (ii). On the other hand, the implication (iii) \Rightarrow (i) can be easily verified and hence, the proof finishes if we show that (ii) implies (iii). Now let G be a bipartite WTD(2) graph, say with parts X and Y . Clearly we will only consider the case when G is not a complete bipartite graph. By definition of X_u and Y_u , note that every dominating edge of G has one endpoint in $X_u \neq \emptyset$ and one endpoint in $Y_u \neq \emptyset$. Moreover, any edge xy where $x \in X_u$ and $y \in Y_u$ is a dominating edge of G .

Therefore, G_{de} is the subgraph of G induced by $X_u \cup Y_u$ and it is complete bipartite. Thus, G_{de} has only two minimal vertex covers, namely X_u and Y_u . Then, definition of a graph in W_2 and Theorem 3.5 imply the existence of the vertices $a \in X \setminus X_u$ and $b \in Y \setminus Y_u$ with $N(a) = Y_u$ and $N(b) = X_u$. \square

Although a polynomial time recognition algorithm for WTD(2) graphs follows from Theorem 2.8, the characterization in Theorem 3.8 provides us with a simple linear time recognition algorithm.

Corollary 3.9. *Triangle-free WTD(2) graphs can be recognized in linear time.*

Proof. Given a graph G , one can check whether it is a connected bipartite graph and if so, find its unique bipartition (X, Y) in linear time (in the number of vertices and edges of G). Then, sets X_u and Y_u can be identified simply by assigning every vertex $x \in X$ such that $d(x) = |Y|$ into X_u , and $y \in Y$ such that $d(y) = |X|$ into Y_u . According to Theorem 3.8, G is triangle-free WTD(2) if and only if either $X_u = X$ and $Y_u = Y$ (thus, G is complete bipartite), or the removal of X_u and Y_u leaves at least one isolated vertex in each one of X and Y . Clearly, all these checks take only linear time. \square

3.3 Planar WTD(2) graphs

In this subsection, we study planar WTD(2) graphs whose minimum degree is at least three and show that such graphs can have at most sixteen vertices. Throughout this section, we frequently use the fact that a graph obtained by an edge contraction of a planar graph is also planar. Recall also that a planar graph contains no K_5 or $K_{3,3}$.

Observation 3.10. *Let G be a WTD(2) graph. The vertex obtained by edge contraction of a dominating edge is a universal vertex in the new graph.*

Let $\nu(G)$ denote the matching number of a graph G .

Lemma 3.11. *Let G be a planar WTD(2) graph. If $\nu(G_{de}) \geq 3$, then $|V(G)| \leq 8$.*

Proof. Suppose that $\nu(G_{de}) \geq 3$ and G has at least 9 vertices. Then, G has three independent dominating edges, say u_1v_1, u_2v_2 and u_3v_3 , and three vertices other than $u_1, u_2, u_3, v_1, v_2, v_3$, say w_1, w_2 and w_3 . Now contract the edges u_1v_1, u_2v_2 and u_3v_3 . In the resulting graph, new three vertices and w_1, w_2, w_3 contain a $K_{3,3}$, which contradicts the planarity. \square

Lemma 3.12. *If G is a WTD(2) graph with $\delta(G) \geq 3$, then $\nu(G_{de}) \geq 2$.*

Proof. Let G be a WTD(2) graph with $\delta(G) \geq 3$. It suffices to show that G has two independent dominating edges. Let xy be a dominating edge of G . Since the minimum degree is at least three, each vertex of G has at least one neighbor in $V(G) \setminus \{x, y\}$. Therefore, $V(G) \setminus \{x, y\}$ is a TDS of G and hence, it contains a dominating edge ab since G is WTD(2). As the dominating edges xy and ab share no vertex, we get $\nu(G_{de}) \geq 2$. \square

Combining the results in Lemmas 3.11 and 3.12 gives the following result.

Proposition 3.13. *If G is a planar WTD(2) graph with $\delta(G) \geq 3$, then $\nu(G_{de}) = 2$ or $|V(G)| \leq 8$.*

We next study planar WTD(2) graphs whose minimum degree is at least 3 and matching number is 2.

Proposition 3.14. *If G is a planar WTD(2) graph with $\delta(G) \geq 3$ and $\nu(G_{de}) = 2$, then $|V(G)| \leq 16$.*

Proof. Let ab and xy be two independent dominating edges of G and $H = G - \{a, b, x, y\}$. Let H_1, \dots, H_m be the connected components of H and order of H_i be h_i for $i = 1, \dots, m$. Note that it suffices to show that $h_1 + \dots + h_m \leq 12$.

We first prove that each H_i is a path or a singleton. Note that it suffices to show that maximum degree of H is at most 2 and H contains no cycle. Suppose that a vertex v of H has three neighbors, say v_1, v_2, v_3 , in H . Then contraction of the edges ab and xy gives rise to a $K_{3,3}$ with parts $\{ab, xy, v\}$ and $\{v_1, v_2, v_3\}$, which is a contradiction. Therefore, every vertex in H has at most two neighbors in H . Suppose that H has a cycle, say v_1, v_2, \dots, v_k . Contract the edge $v_k v_{k-1}$ and denote the new point by v_{k-1} . Then contract the edge $v_{k-1} v_{k-2}$ and denote the new point by v_{k-2} and so on. Follow this process until we get a triangle v_1, v_2, v_3 . Then contracting the edges ab and xy yields a K_5 with vertices ab, xy, v_1, v_2, v_3 , which is a contradiction. Thus, H has no cycle and hence, H is a disjoint union of paths and singletons.

We next show that for every vertex $u \in H$ we have $|N(u) \cap \{a, b, x, y\}| \geq 3$ or $|(N(u) \cup N(v)) \cap \{a, b, x, y\}| \geq 3$ for some neighbor $v \in V(H)$ of u . Since both ab and xy are dominating edges, the intersection $N(u) \cap \{a, b, x, y\}$ has at least two elements: one from $\{a, b\}$ and one from $\{x, y\}$. Consider the case when $|N(u) \cap \{a, b, x, y\}| = 2$. Without loss of generality, let $N(u) \cap \{a, b, x, y\} = \{a, x\}$. Since the minimum degree of G is at least 3, there is no vertex $v \in G$ such that $N(v) = \{a, x\}$. Hence, by Proposition 3.2 the set $\{a, x\}$ is not a vertex cover of G_{de} . Then, there exists an edge wv of G_{de} such that $\{w, v\} \cap \{a, x\} = \emptyset$. Thus, as $\nu(G_{de}) = 2$ and $ab, xy \in G_{de}$, we have $wv = by$ or $w \in \{b, y\}$ and $v \in V(H)$. Recall that wv is a dominating edge in G and hence, u is adjacent to w or v . Therefore, the case $wv = by$ is impossible and we see that v is adjacent to u . Consequently, we get $|(N(u) \cup N(v)) \cap \{a, b, x, y\}| \geq 3$ since $w \in \{b, y\}$ is a neighbor of v . Note that this result implies that if $\{u\}$ is a component of H , then u has at least three neighbors among a, b, x, y ; otherwise, contraction of the edge uv gives rise to a vertex adjacent to at least three of a, b, x, y .

We then apply the following process for each $i = 1, \dots, m$: If $h_i \leq 3$, contract the edges of H_i and obtain a singleton. If $h_i \geq 4$, let H_i be the path v_1, v_2, \dots, v_k where $k = h_i$. First, contract $v_1 v_2$ and $v_{k-1} v_k$. Then contract the paths $v_3 v_4 v_5, v_6 v_7 v_8, \dots$ and so on. Note that for every i we obtain at least $2 + \lfloor (h_i - 4)/3 \rfloor = \lfloor (h_i + 2)/3 \rfloor$ vertices adjacent to at least three of a, b, x, y . Therefore, each such vertex is adjacent to both a and b or adjacent to both x and y . Assume that the number of vertices having at least three neighbors among a, b, x, y in the resulting graph is more than 4. Then, by pigeonhole principle, there will be three distinct vertices u_1, u_2 and u_3 each of which is adjacent, without loss of generality, to both a and b . Then, contraction of the edge xy gives a $K_{3,3}$ with parts $\{a, b, xy\}$ and $\{u_1, u_2, u_3\}$, contradicting the planarity of G . Thus, there are at most 4 vertices having at least three neighbors among a, b, x, y once the contraction process is terminated, that is, $\sum_{i=1}^m \lfloor (h_i + 2)/3 \rfloor \leq 4$. Since h_i is an integer, the inequality $h_i/3 \leq \lfloor (h_i + 2)/3 \rfloor$ holds, implying that $\sum_{i=1}^m h_i/3 \leq 4$ which yields $\sum_{i=1}^m h_i \leq 12$ as desired. \square

Propositions 3.13 and 3.14 imply that, unlike the general case stated in Corollary 2.5, there is a finite number of planar WTD(2) graphs with $\delta(G) \geq 3$.

Theorem 3.15. *If G is a planar WTD(2) graph with $\delta(G) \geq 3$, then $|V(G)| \leq 16$.*

In contrast, there is no upper bound on the number of vertices for planar WTD(2) graphs with minimum degree 1 or 2. For example, consider a star with arbitrarily many leaves and a graph with arbitrarily many triangles sharing a common edge, respectively.

4 Girth of WTD graphs

In this section, we provide a relation between the minimum degree and the girth for WTD graphs. We show that if the minimum degree is more than two in a WTD graph, then the graph contains a cycle of length at most twelve. It is shown in [12] that if G is a WTD graph with $\delta(G) \geq 2$, then the girth of G , $g(G)$, is at most 14.

Theorem 4.1 ([12, Theorem 4.1]). *Suppose G is a connected graph with no leaves such that G has girth at least fifteen. Then $\gamma_t(G) < \Gamma_t(G)$.*

By following the idea in the proof of Theorem 4.1 in [12], one can find other relations between $\delta(G)$ and $g(G)$ of a WTD graph G . Before presenting such extensions, we need the following useful lemma, which is also given in [12]:

Lemma 4.2. *Let G be a WTD graph, u_1v_1, \dots, u_mv_m be a subset of the edges of G and $A = \cup_{i=1}^m \{u_i, v_i\}$. If the subgraph of G induced by A is disjoint union of m complete graphs of order 2 and $G - N[A]$ has no isolated vertices, then $G - N[A]$ is also WTD.*

Proof. Let S be a minimal TDS of $G - N[A]$. We claim that $S \cup A$ is a minimal TDS of G . It is easy to see that it is a TDS of G . Suppose that $S \cup A$ contains another TDS of G , say T . Then $T \cap S$ is a TDS of $G - N[A]$ and hence, since S is minimal we get $T \cap S = S$. Therefore, we obtain $T = S \cup A'$ where $A' \subseteq A$. If $A \setminus A'$ is nonempty, then without loss of generality we assume that $u_1 \in A \setminus A'$. But then, v_1 is not dominated by T , which is a contradiction. Therefore, we have $A' = A$, which implies that $T = S \cup A$, that is, $S \cup A$ is minimal.

As every minimal TDS of G has the same size, $|S| + 2m$ is independent of S and hence, $G - N[A]$ is a WTD graph as well. □

Theorem 4.3. *If G is a WTD graph with $\delta(G) \geq 3$, then $g(G) \leq 12$.*

Proof. Assume that G is a WTD graph with $\delta(G) \geq 3$ and $g(G) \geq 13$. Let $P = v_1, v_2, v_3, v_4, v_5$ be a path in G . For any vertex v in G , let $d_P(v) = \min_{1 \leq i \leq 5} \text{dist}(v, v_i)$. Define N_k to be the set of vertices v with $d_P(v) = k$ for $k = 1, 2, \dots$.

First note that every vertex in N_k has a neighbor in N_{k-1} for every $k \geq 2$. Moreover, for $k = 1, 2, 3$, N_k is an independent set since otherwise we obtain a cycle of length at most 11. We will now show that for $k = 1, \dots, 4$, any vertex in N_k has at least one neighbor in N_{k+1} . Suppose that there exist $k \leq 4$ and $v \in N_k$ such that v is adjacent to no vertex in N_{k+1} . By definition, it is clear that v has no neighbor in N_l for any $l \geq k + 2$. Therefore, all the neighbors of v are in $\cup_{1 \leq i \leq k} N_i$. Thus, as v has at least three neighbors, there exist three paths from v to P such that one of them has length k and two of them have length at most $k + 1$. By a simple case analysis, considering the vertices of these paths on P gives that there exist a cycle of length at most $2k + 3 \leq 11$, which is a contradiction.

Now, let $N_2 = \{w_1, \dots, w_m\}$. For every $i = 1, \dots, m$, choose a neighbor of w_i in N_3 , say u_i . Let $A = \cup_{i=1}^m \{w_i, u_i\}$. For any $i \neq j$, w_i is not adjacent to u_j because otherwise we obtain a cycle of length at most 10. Therefore, the induced subgraph of G induced by A is a disjoint union of m complete graphs of order 2.

Next, consider the graph $H = G - N[A]$. Note that $N[A]$ consists of N_1, N_2, N_3 and some vertices in N_4 . Therefore, P is a connected component of H . As any vertex in N_4 has a neighbor in N_5 , no vertex $v \in N_4 \cap V(H)$ is isolated in H . Clearly, no vertex in N_k with $k \geq 6$ is isolated in H since it has a neighbor in N_{k-1} . Suppose to the contrary that a vertex v in N_5 is isolated in H . Then v has no neighbor in N_5 and N_6 , and thus, all its neighbors are in N_4 . Therefore, since there exist three paths from v to P , this yields a cycle of length at most 12, which is a contradiction. Consequently, H has no isolated vertices and we can apply Lemma 4.2 and conclude that H is a WTD graph. However, P is a component of H and hence, it should be WTD as well. Nevertheless, a path of length 4 is not a WTD graph (both $\{v_1, v_2, v_4, v_5\}$ and $\{v_2, v_3, v_4\}$ are minimal TDSs of P), which is a contradiction. \square

5 Conclusion

In this work, we studied graphs whose all minimal total dominating sets have the same size. We say these graphs are well-totally-dominated. We proved that well-totally-dominated graphs with bounded total domination number can be recognized in polynomial time. We then analyzed well-totally-dominated graphs with total domination number two for the special cases of triangle-free graphs and planar graphs. Finally, we focused on the girth of well-totally-dominated graphs. In particular, we proved that a well-totally-dominated graph with minimum degree at least three has girth at most 12. We now conclude with several future research directions.

Although we proved in this paper that the problem of recognizing well-totally-dominated graphs with bounded total domination number can be solved in polynomial time, the complexity of the general case is an open research problem. Hence, we pose the following question:

Problem 5.1. What is the computational complexity of recognizing well-totally-dominated graphs?

We have already characterized WTD(2) graphs with packing number $\rho(G) = 2$ in Theorem 3.5. Since WTD(2) graphs have $\rho(G) \leq 2$, in order to complete the characterization of all WTD(2) graphs, it remains to answer the following question:

Problem 5.2. What are WTD(2) graphs with $\rho(G) = 1$?

Along the same line, one may consider to generalize our result in Theorem 3.5. It is well known that $\rho(G) \leq \gamma_t(G) \leq \Gamma_t(G)$; hence graphs with $\rho(G) = \Gamma_t(G)$ form a subclass of WTD graphs. This suggests our next open problem:

Problem 5.3. What are WTD(k) graphs with $\rho(G) = k$?


Lastly, we have shown in Theorem 3.15 that planar WTD(2) graphs with $\delta(G) \geq 3$ have at most 16 vertices. Our intuition is that 16 is not a tight bound. Thus, we pose the following question:

Problem 5.4. Is the upper bound of 16 for the number of vertices of a planar WTD(2) graph with $\delta(G) \geq 3$ tight? Can we determine all (finitely many) planar WTD(2) graphs?

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Nordhaus-Gaddum type inequalities for the distinguishing index

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Abstract

The distinguishing index of a graph G , denoted by $D'(G)$, is the least number of colours in an edge colouring of G not preserved by any nontrivial automorphism. This invariant is defined for any graph without K_2 as a connected component and without two isolated vertices, and such a graph is called admissible. We prove the Nordhaus-Gaddum type relation:

$$2 \leq D'(G) + D'(\overline{G}) \leq \Delta(G) + 2$$

for every admissible connected graph G of order $|G| \geq 7$ such that \overline{G} is also admissible.

Keywords: Symmetry breaking in graphs, distinguishing index, Nordhaus-Gaddum type bounds.

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1 Introduction and main result

We consider finite graphs and their edge colourings, not necessarily proper. Such a colouring *breaks an automorphism* of a graph if there exists an edge that is mapped into an edge with a different colour by that automorphism. A colouring is called *asymmetric* (or *distinguishing*), if it breaks all non-trivial automorphisms. The minimum number of colours in an asymmetric colouring of a graph G is called the *distinguishing index* of G and is denoted by $D'(G)$. Obviously, the distinguishing index is defined only for graphs without K_2 as a component and with at most one isolated vertex. We call such graphs *admissible*.

The following general upper bound for the distinguishing index of connected graphs with respect to the maximum degree was proved by Kalinowski and Piłśniak in [8].

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Theorem 1.1 ([8]). *If G is a connected graph with at least three vertices, then*

$$D'(G) \leq \Delta(G)$$

unless G is C_3 , C_4 or C_5 .

This result was improved in [10], where all connected graphs with the distinguishing index equal to the maximum degree were characterized. In particular, a tree is called *symmetric* (respectively, *bisymmetric*) if it contains a central vertex v_0 (resp. a central edge e_0), all leaves are at the same distance from v_0 (resp. e_0) and all vertices that are not leaves have the same degree.

Theorem 1.2 ([10]). *Let G be a connected graph of order at least three. Then*

$$D'(G) \leq \Delta(G) - 1$$

unless G is a cycle, a symmetric or a bisymmetric tree, K_4 or $K_{3,3}$.

In the same paper, the conjecture for 2-connected graphs was formulated, and quite recently was confirmed in [7] in a bit stronger form, as follows.

Theorem 1.3 ([7]). *If G is a connected graph with minimum degree $\delta(G) \geq 2$, then*

$$D'(G) \leq \left\lceil \sqrt{\Delta(G)} \right\rceil + 1.$$

The main goal of the paper is a proof of a Nordhaus-Gaddum type inequalities for the distinguishing index of a graph. Our investigation was motivated by the renowned result of Nordhaus-Gaddum [9] who determined in 1956 lower and upper bounds for the sum of the chromatic numbers of a graph and its complement (actually, the upper bound was first proved by Zykov [12] in 1949). Since then, Nordhaus-Gaddum type bounds were obtained for many graph invariants. An exhaustive survey is given in [1]. In particular, it was considered by Collins and Trenk in [3] for the distinguishing chromatic number $\chi_D(G)$, which is the minimum number of colours in an asymmetric proper vertex colouring of a graph G . The Nordhaus-Gaddum type inequalities were also investigated in [10] for the chromatic distinguishing index $\chi'_D(G)$ of a graph G defined for asymmetric proper edge colourings. It was proved therein that if G is an admissible graph of order $n \geq 3$ distinct from $K_{1,4}$, then

$$n - 1 \leq \chi'_D(G) + \chi'_D(\overline{G}) \leq 2(n - 1).$$

Both upper and lower bounds are similar to Vizing bounds proved for the chromatic index of a graph [11] but in the proof for the chromatic distinguishing index we have to be more careful.

It was also conjectured in [10] that

$$2 \leq D'(G) + D'(\overline{G}) \leq \max\{\Delta(G), \Delta(\overline{G})\} + 2$$

if both graphs G and \overline{G} are admissible and of order $n \geq 7$. It was confirmed for some classes of graphs, in particular for trees, claw-free graphs, 3-connected graphs and traceable graphs. Here, we prove the stronger version of Nordhaus-Gaddum type inequality for the distinguishing index.

Theorem 1.4 (Main Theorem). *If both G and \overline{G} are admissible graphs of order $n \geq 7$, and G is connected, then*

$$2 \leq D'(G) + D'(\overline{G}) \leq \Delta(G) + 2.$$

The lower bound by 2 is obvious. Indeed, if a graph G is *asymmetric*, that means it has a trivial automorphism group, then the distinguishing index of both G and \overline{G} equals 1. Moreover, Theorem 1.4 is tight. To see this, consider a symmetric (or bisymmetric) tree T of order $n \geq 7$. Then by [5] \overline{T} contains an asymmetric spanning tree if T is different from a star, so $D'(\overline{T}) = 2$ by Proposition 2.2. So, it follows from Theorem 1.2 that $D'(T) + D'(\overline{T}) = \Delta(T) + 2$ for symmetric and bisymmetric trees.

It has to be noted that there exist graphs of order less than 7 violating the right inequality in Theorem 1.4. For example, $D'(K_{3,3}) = 3$, $D'(\overline{K_{3,3}}) = 4$, whence $D'(K_{3,3}) + D'(\overline{K_{3,3}}) = \Delta(K_{3,3}) + 4$. Also, $D'(C_5) + D'(\overline{C_5}) = \Delta(C_5) + 4$, and $D'(K_{1,i}) + D'(\overline{K_{1,i}}) = \Delta(K_{1,i}) + 3$ for $i = 3, 4, 5$.

In Section 2 we recall some results useful in the proof of Theorem 1.4, which is given in Section 3.

2 Known bounds for D'

Let us recall some useful results, before we start to prove the Main Theorem. A graph that contains a Hamiltonian path, i.e. a path that visits each vertex of the graph, is called *traceable*. Following [2], we define the k -th *Bondy-Chvátal closure* $cl_k(G)$ of a graph G as the graph obtained from G by recursively joining pairs of non-adjacent vertices with degree-sum at least k . By the well-known theorem of Bondy and Chvátal [2], a graph G of order n is traceable whenever $cl_{n-1}(G)$ is traceable.

We begin with the distinguishing index of complete graphs and of traceable graphs.

Proposition 2.1 ([8]).

$$D'(K_n) = \begin{cases} 2, & \text{if } n \geq 6, \\ 3, & \text{if } n = 3, 4, 5. \end{cases}$$

The following simple observation is very useful in some proofs. A subgraph H of a graph G is called *almost spanning* if H is a spanning subgraph of a graph $G - v$ for some $v \in V(G)$.

Proposition 2.2 ([10]). *If H is a spanning or almost spanning subgraph with at least three vertices of a graph G , then $D'(G) \leq D'(H) + 1$.*

In particular, the spanning path in a traceable graph needs two colours to break its non-trivial automorphism, so a traceable graph has the distinguishing index at most 3. Actually we have a stronger result.

Theorem 2.3 ([10]). *Let G be a traceable graph of order at least 3. If G has at least 7 vertices, then $D'(G) \leq 2$. Moreover, if G is of order at most 6, then $D'(G) \leq 3$.*

The distinguishing index of complete bipartite graphs was determined independently by Fisher and Isaak [4] and by Imrich, Jerebic and Klavžar [6]. Actually, they formulated their result for the distinguishing number $D(K_p \square K_q)$ of the Cartesian product of complete graphs, but $D'(K_{p,q}) = D(K_p \square K_q)$.

Theorem 2.4 ([4, 6]). *Let p, q, d be integers such that $d \geq 2$ and $(d - 1)^p < q \leq d^p$. Then*

$$D'(K_{p,q}) = \begin{cases} d, & \text{if } q \leq d^p - \lceil \log_d p \rceil - 1, \\ d + 1, & \text{if } q \geq d^p - \lceil \log_d p \rceil + 1. \end{cases}$$

If $q = d^p - \lceil \log_d p \rceil$, then the distinguishing index $D'(K_{p,q})$ is either d or $d + 1$ and can be computed recursively in $O(\log^(q))$ time.*

In the rest of the paper, we make use of the following immediate corollary.

Corollary 2.5. *If $p \leq q$, then $D'(K_{p,q}) \leq \lceil \sqrt[p]{q} \rceil + 1$.*

The following simple observation is used later in this section.

Proposition 2.6. *If H is an admissible disconnected graph of order at least 7, then $D'(H) \leq |H| - 2$.*

Proof. Theorem 1.2 implies that the only connected graph H with $D'(H) \geq |H| - 1$ is K_3, K_4, C_4 or a star $K_{1,n-1}$ for $n \geq 3$. If all components H_1, \dots, H_s of H are pairwise non-isomorphic, then $D'(H) = \max\{D'(H_i) : i = 1, \dots, s\}$, so $D'(H) \leq |H| - 2$. If H contains $t \geq 2$ copies of a graph H_1 as its components, so $|H| \geq t|H_1|$, then we colour one of them distinguishingly and use one extra colour for each other copy. Hence,

$$D'(tH_1) \leq D'(H_1) + t - 1 \leq |H_1| + t - 1 \leq \frac{|H|}{t} + t - 1 \leq |H| - 2. \quad \square$$

We easily extend a result of [10] for trees to forests. First, recall a result of Hedetniemi et al. [5] on packing two trees into K_n .

Theorem 2.7 ([5]). *A complete graph K_n contains edge disjoint copies of any two trees of order n distinct from a star $K_{1,n-1}$.*

Proposition 2.8. *Let G be an admissible graph of order n such that \overline{G} is an admissible forest. Then $D'(G) \leq 2$ if $n \geq 7$, and $D'(G) \leq 3$ otherwise.*

Proof. The case when \overline{G} is a tree was proved in [10]. Otherwise, it easily follows from Theorem 2.7 that G contains a Hamiltonian path P_n . Indeed, we can consider a tree F' spanned by \overline{G} , and every tree distinct from a star is included in a subgraph $\overline{F'}$ of G . Thus $D'(G) \leq 2$ if $n \geq 7$, and $D'(G) \leq 3$ if $3 \leq n \leq 6$ by Theorem 2.3. \square

Additionally, let us note the following observation for small graphs. Denote by W_1 and W_2 the two graphs from Figure 1 called *windmills*.

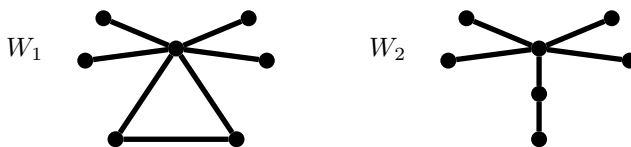


Figure 1: Two windmills.

Proposition 2.9. *If G is a connected graph of order at most 7 different from windmills W_1 and W_2 , and from a star $K_{1,n}$ for $n = 4, 5, 6$, then $D'(G) \leq 3$.*

Proof. Observe that if $\Delta(G) \leq 4$, then the claim holds by Theorem 1.2. So let $\Delta(G) \geq 5$. First assume that G does not have pendant edges. If the longest cycle in G is of order at least 6, then G is traceable and $D'(G) \leq 3$ by Theorem 2.3. If the longest cycle C in G is of order 5, then we colour the edges of this cycle with 0, 1, 0, 2, 0 (in this order) and all chords with 1. Thus, each vertex of C has an incident edge coloured with 0. If there exists a vertex of G with noncoloured incident edges, then all of them we colour with 2 and all the remaining edges with 1. It is an asymmetric colouring of G , because outside the initial cycle C we create a monochromatic vertex with colour 2 and a monochromatic vertex with colour 1 or a bichromatic one with colours 1 and 2.

If the longest cycle in G is of order 4, then a 2-connected G is isomorphic to $K_{2,r}$ or $K_{2,r} + e$ with $r \leq 5$ where e is an edge between two vertices of maximum degree. Three colour suffice for an asymmetric colouring of r paths of length two between the two vertices of maximum degree. If such a 2-connected graph is joined with a triangle (in a cut vertex), then we can colour every edge of the triangle with a different colour. If two cycle of length 4 (with chords) meet in only one vertex, then an asymmetric colouring of one of them uses colour 1 twice, while the other one uses 2 twice (apart from one edge coloured with 0).

If the longest cycle is a triangle C_3 , then G has a cut vertex v where three cycles meet. Then a pair of edges including v in every triangle is coloured with 1 and 2, while every remaining edge obtains a distinct colour 1, 2 or 3.

Now assume that there exists a leaf v in G . First suppose there exists an induced subgraph B of G with minimal degree at least 2. Then we can colour it with three colours as above. So we have to distinguish now only pendant trees (in particular paths and edges) with a common vertex just fixed in B . It is always possible to do this with three colours if $|G| \leq 7$ unless B has a pendant star $K_{1,4}$. Then we obtain an exceptional graph W_1 .

Finally, let G be a tree of order at most 7 different from a star $K_{1,n}$ with $n = 3, \dots, 6$. Then $D'(G) \leq \Delta(G) - 1$ by Theorem 1.2. Clearly, $D'(G) \leq 3$ unless $G = W_2$, which needs four colours like W_1 . □

3 Proof of the Main Theorem

Proof of Theorem 1.4. Let G be a connected graph of order $n \geq 7$ such that both G and its complement \overline{G} are admissible. Denote $\Delta = \Delta(G)$. Clearly, $\Delta \geq \Delta(\overline{G}) + 1$ whenever \overline{G} is disconnected. Next, if $\Delta \leq \frac{n-1}{2}$, then

$$\delta(\overline{G}) = n - 1 - \Delta \geq \frac{n-1}{2},$$

and \overline{G} is connected. Otherwise, $\frac{n-1}{2} \geq \Delta \geq \Delta(\overline{G}) + 1 \geq \frac{n-1}{2} + 1$. Hence, \overline{G} satisfies the well-known Dirac's condition for traceability, so \overline{G} is traceable. Hence, $D'(G) + D'(\overline{G}) \leq \Delta + 2$ by Theorem 1.1 and Theorem 2.3.

Assume then that $\Delta \geq \lceil \frac{n}{2} \rceil$. Analogously, we can assume that $\Delta(\overline{G}) \geq \lceil \frac{n}{2} \rceil$. Indeed, our theorem holds if $\Delta(\overline{G}) \leq \frac{n-1}{2}$. Then $D'(G) \leq 2$ and $D'(\overline{G}) \leq \Delta(\overline{G}) \leq \frac{n-1}{2} \leq \Delta$ if \overline{G} is connected, or $D'(\overline{G}) \leq \lceil \frac{n}{2} \rceil \leq \Delta$ if \overline{G} is disconnected, by the following reasons.

Theorem 1.1 implies that the only connected graphs H with $D'(H) > \Delta(H)$ are C_3, C_4 and C_5 . If all components H_1, \dots, H_s of \overline{G} are pairwise non-isomorphic, then

$D'(\overline{G}) = \max\{D'(H_i) : i = 1, \dots, s\} \leq \max\{3, \Delta(H_i)\}$, so $D'(\overline{G}) \leq \frac{n}{2}$. If \overline{G} contains $t_i \geq 2$ copies of a graph H_i as its components, then let $t = \max\{t_i : i = 1, \dots, s\}$ and let $H = H_t$ where $D'(H_t) = \max\{D'(H_i) : i = 1, \dots, s\}$, and we colour one copy of H_t distinguishingly and use one extra colour for each other copy. So, for H different from C_3, C_4 and C_5 we have

$$D'(\overline{G}) \leq D'(tH_t) \leq D'(H_t) + t - 1 \leq \Delta(H_t) + t - 1 \leq \frac{|\overline{G}|}{t} + t - 2 \leq \frac{n}{2},$$

and for $i \in \{3, 4, 5\}$ we obtain $D'(tC_i) \leq t + 2 \leq \lceil \frac{ti}{2} \rceil$.

We distinguish two cases.

Case A: Both G and \overline{G} are connected graphs without pendant edges.

Then $D'(G) \leq \lceil \sqrt{\Delta} \rceil + 1$ and $D'(\overline{G}) \leq \lceil \sqrt{\Delta(\overline{G})} \rceil + 1$. Hence, the inequality $D'(G) + D'(\overline{G}) \leq \Delta + 2$ is weaker than

$$\Delta - \lceil \sqrt{\Delta} \rceil \geq \lceil \sqrt{\Delta(\overline{G})} \rceil. \tag{3.1}$$

First assume that $\Delta \geq \Delta(\overline{G})$. It is easy to see that the inequality (3.1) is satisfied unless $\Delta = \Delta(\overline{G}) = 5$. In the latter case $8 \leq n \leq 10$ and $\delta(G) = \delta(\overline{G}) = n - 6$. We want to show that either G or its complement \overline{G} is traceable.

We say that a sequence (a_i) is minorized by a sequence (b_i) if $b_i \leq a_i$ for any i . If $n = 8$, then the degree sequence, ordered non-increasingly, of G (or \overline{G}) is minorized by $(5, 5, 4, 4, 2, 2, 2, 2)$ or by $(5, 4, 4, 4, 3, 2, 2, 2)$. Indeed, we know by assumptions that $b_1 = 5, b_8 = 2$, two terms of b_i have to be odd since the sum of degrees is even in every graph, and the sum of the fourth term of the sequence of G and the fifth term of the sequence of \overline{G} equals $n - 1 = 7$, so one of them cannot be smaller than $\lceil \frac{n-1}{2} \rceil = 4$. Now, by definition of the $(n - 1)$ -th Bondy-Chvátal closure $cl_{n-1}(G)$, a vertex of degree five in G has degree $n - 1 = 7$ in $cl_7(G)$, so we have to add two new edges incident to it. Observe that adding new edges yields another vertex that has degree $n - 1$ in $cl_7(G)$, and this is the case at each step of creating $cl_7(G)$. Finally, $cl_7(G) = K_8$. Hence, G is traceable, by the Bondy-Chvátal theorem [2].

Similarly, if $n = 9$, we may assume that the degree sequence of G is minorized by $(5, 4, 4, 4, 4, 3, 3, 3)$ or by $(5, 5, 4, 4, 4, 3, 3, 3)$, and it is not difficult to see that $cl_8(G) = K_9$. For $n = 10$, the degree sequence of G is minorized by $(5, 5, 4, \dots, 4)$ and here it is clear that $cl_9(G) = K_{10}$. For brevity, the details are left to the reader.

Now assume that $\Delta(\overline{G}) > \Delta$. Then it is easily seen that the inequality (3.1) holds for any $\Delta, \Delta(\overline{G})$ and n unless either $n = 8, \Delta = 4, \Delta(\overline{G}) = 5$, or $n = 9, \Delta = 5, \Delta(\overline{G}) = 6$, or $n = 10, \Delta = 5, \Delta(\overline{G}) \in \{6, 7\}$, since $\lceil \frac{n}{2} \rceil - \lceil \sqrt{\lceil \frac{n}{2} \rceil} \rceil \geq \lceil \sqrt{n - 3} \rceil$. The same argument as above confirms that \overline{G} is traceable.

Case B: A graph \overline{G} is disconnected or $\delta(\overline{G}) = 1$.

If \overline{G} is a forest, then the conclusion follows from Proposition 2.8. Hence, assume that \overline{G} contains a 2-connected block. We now consider decompositions of \overline{G} into two subgraphs F_1, F_2 such that $E(F_1) \cup E(F_2) = E(\overline{G})$ and the vertex sets $V(F_1), V(F_2)$ share at most one vertex which is a cut-vertex of \overline{G} . Denote $p = |F_1| - 1, q = |F_2| - 1$ if F_1 and F_2 share a common vertex, and $p = |F_1|, q = |F_2|$ if F_1 and F_2 are disjoint. Assume that $p \leq q$ and the difference $q - p$ is smallest possible. Observe that $\Delta(G) \geq q$ and G is spanned or almost spanned by a complete bipartite graph $K_{p,q}$.

First, suppose that $q \leq 2^p - p$. Then $D'(G) \leq 2$, since G is (almost) spanned by an asymmetric spanning subgraph of $K_{p,q}$ for $p + q \geq 7$ by Proposition 3.10 in [10] (see also [6]).

If \overline{G} is connected, then $\Delta = \Delta(G) = n - 2$ since $\delta(\overline{G}) = 1$ by the assumption of Case B. Moreover, $D'(\overline{G}) \leq n - 2$ by Theorem 1.1 as $\Delta(\overline{G}) \leq n - 2$. Hence

$$D'(G) + D'(\overline{G}) \leq 2 + n - 2 = \Delta + 2.$$

If \overline{G} is disconnected, then either $\delta(\overline{G}) = 1$ or $\delta(\overline{G}) \geq 2$. If $\delta(\overline{G}) = 1$, then $D'(\overline{G}) \leq n - 2$ by Proposition 2.6 and $D'(G) + D'(\overline{G}) \leq 2 + n - 2 = \Delta + 2$. Now, let $\delta(\overline{G}) \geq 2$, and assume (in the worst case) that \overline{G} contains s components isomorphic to a connected graph H . Recall that $\Delta(\overline{G}) \geq \frac{n}{2}$, as we assumed at the beginning of the proof. So, $3 \leq |H| < \frac{n}{2s}$. If we use a distinct additional colour for every component H , then $D'(\overline{G}) \leq \lceil \sqrt{\Delta(\overline{G})} \rceil + s \leq \lceil \sqrt{n-2} \rceil + s$, by Theorem 1.3. So, we would like to show that

$$\lceil \sqrt{n-2} \rceil + s + 2 \leq n - |H| + 2, \tag{3.2}$$

since $\Delta(G) \geq n - |H|$. To confirm the inequality (3.2), we estimate

$$\lceil \sqrt{n-2} \rceil + s \leq \lceil \sqrt{n-2} \rceil + \frac{n}{6} \leq n - \frac{n}{4} \leq n - |H|.$$

It is easy to verify that the second inequality is always true. The last inequality is obvious if s is at least 2. If $s = 1$ we do not need to distinguishing connected component one from another, hence we use the same colours in every component and $D'(\overline{G}) \leq \lceil \sqrt{\Delta(\overline{G})} \rceil + 1 \leq \Delta$. So, this subcase is completed.

Now, assume that $q \geq 2^p - p + 1$. Then $D'(G) \leq \sqrt[p]{q} + 2$ for $p \geq 2$ by Corollary 2.5 and Proposition 2.2. In this case the graph \overline{G} can be obtained from a 2-connected graph B by attaching a number of independent pendant subgraphs (of order at most p) to it or there is a component of order p and a 2-connected component B of order q . Hence, $\Delta(B) \leq q$ and $D'(\overline{G}) \leq \lceil \sqrt[q]{q} \rceil + 1$, by Theorem 1.3 for the block B , and by the observation that then every subgraph attached to B has one vertex fixed and the order at most $p \leq \sqrt[q]{q} + 2$. We obtain $D'(G) + D'(\overline{G}) \leq \lceil \sqrt[p]{q} \rceil + 2 + \lceil \sqrt[q]{q} \rceil + 1$. Recall that $\Delta \geq q$, so it is enough to check whether

$$\lceil \sqrt[p]{q} \rceil + \lceil \sqrt[q]{q} \rceil + 3 \leq q + 2.$$

Consequently, we obtain the inequality

$$q - \lceil \sqrt[p]{q} \rceil - \lceil \sqrt[q]{q} \rceil - 1 \geq 0. \tag{3.3}$$

For $p = 3$, we have $q \geq 2^3 - 3 + 1 = 6$. For $q = 6, p = 3$ we have $D'(G) \leq 4$ by Proposition 2.2, and $D'(\overline{G}) \leq 3$ by Proposition 2.9 for F_2 . Observe now that the inequality (3.3) is satisfied, because it holds for $q = 7$, and $q - \lceil \sqrt[3]{q} \rceil - \lceil \sqrt[q]{q} \rceil - 1$ is an increasing function of q . The inequality (3.3) also holds for larger values of p since its left-hand side is non-decreasing with respect to p .

If $p = 2$, then inequality (3.3) is satisfied for $q \geq 7$. For $q = 5$ or $q = 6$, G is (almost) spanned by $K_{2,5}$ or $K_{2,6}$, so $D'(G) \leq 4$ by Proposition 2.2, and $D'(\overline{G}) \leq 3$ by Proposition 2.9 for F_2 . For $q = 4$ we have $n = 7$ and our theorem is true by Proposition 2.9.

Now let $p = 1$. If \overline{G} is disconnected, then \overline{G} contains a 2-connected block B of order $n - 1$ and an isolated vertex v . Hence, $\Delta = n - 1$, of course. Then $D'(\overline{G}) \leq D'(B) \leq$

$\lceil \sqrt{\Delta(\overline{G})} \rceil + 1$. Moreover, $D'(G) \leq \lceil \sqrt{\Delta} \rceil + 1$ whenever $\delta(G) \geq 2$, by Theorem 1.3. Hence,

$$D'(G) + D'(\overline{G}) \leq 2\lceil \sqrt{\Delta} \rceil + 2,$$

and $2\lceil \sqrt{\Delta} \rceil + 2 \leq \Delta + 2$ for $\Delta \geq 6$, since $\Delta = n - 1 \geq 6$.

If the graph \overline{G} is connected, then \overline{G} can be obtained from a 2-connected block B by attaching a number (maybe zero) of independent pendant edges to it. It is enough to break all nontrivial automorphisms of B . Then $D'(\overline{G}) \leq D'(B) \leq \lceil \sqrt{\Delta(\overline{G})} \rceil + 1$. Moreover, $\Delta = n - 2$ and $D'(G) \leq \lceil \sqrt{\Delta} \rceil + 1$ whenever $\delta(G) \geq 2$, by Theorem 1.3. Then $2\lceil \sqrt{\Delta} \rceil + 2 \leq \Delta + 2$ for $\Delta \geq 6$, unless $\Delta = 5$. But in the latter case $n = 7$ and $D'(G) + D'(\overline{G}) \leq 6$ by Proposition 2.9.

Finally, assume that $p = 1$ and $\delta(G) = 1$. Then we consider decompositions of G into two subgraphs F'_1, F'_2 such that $E(F'_1) \cup E(F'_2) = E(G)$ and the vertex sets $V(F'_1), V(F'_2)$ share one vertex which is a cut-vertex of G . Denote $p' = |F'_1| - 1, q' = |F'_2| - 1$. Assume that $p' \leq q'$ and the difference $q' - p'$ is smallest possible. Recall that $\Delta(\overline{G}) = n - 2$ and \overline{G} is spanned or almost spanned by a complete bipartite graph $K_{p',q'}$.

If $q' \leq 2^{p'} - p'$, then $D'(\overline{G}) \leq 2$ like above (for $p' + q' \geq 7$), and $D'(G) \leq \Delta$ by Theorem 1.1. So, we are done. If $q' \geq 2^{p'} - p' + 1$, then $D'(\overline{G}) \leq \sqrt[p']{q'} + 2$ for $p' \geq 2$, and we obtain

$$D'(G) + D'(\overline{G}) \leq \lceil \sqrt{q'} \rceil + \lceil \sqrt[p']{q'} \rceil + 3 \leq p' + q' + 1,$$


since $\Delta \geq n - 2 = p' + q' - 1$. For $p' = 2$, we have $q' \geq 2^2 - 2 + 1 = 3$, and the inequality $2\lceil \sqrt{q'} \rceil \leq q'$ is satisfied since $n \geq 7$. Hence $q' \geq 4$. The inequality $p' + q' - \lceil \sqrt{q'} \rceil - \lceil \sqrt[p']{q'} \rceil - 2 \geq 0$ also holds for larger values of p' since its left-hand side is non-decreasing with respect to p' .

Let $p' = 1$. Then there exists a 2-connected block B' in G with a number of independent pendant edges attached to it (at least one). Hence $D'(G) \leq D'(B') \leq \lceil \sqrt{\Delta} \rceil + 1$. Recall that also $D'(\overline{G}) \leq \lceil \sqrt{\Delta(\overline{G})} \rceil + 1 \leq \lceil \sqrt{\Delta} \rceil + 1$, since $\Delta = \Delta(\overline{G}) = n - 2$. So we verify the following inequality

$$2\lceil \sqrt{\Delta} \rceil + 2 \leq \Delta + 2$$

for $\Delta \in \{n - 2, n - 1\}$, which is true for $n \geq 7$ unless $\Delta = 5$. But then $n = 7$ and $D'(G) + D'(\overline{G}) \leq 6$ once more by Proposition 2.9. □

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Closed formulas for the total Roman domination number of lexicographic product graphs

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Abstract

Let G be a graph with no isolated vertex and $f: V(G) \rightarrow \{0, 1, 2\}$ a function. Let $V_i = \{x \in V(G) : f(x) = i\}$ for every $i \in \{0, 1, 2\}$. We say that f is a total Roman dominating function on G if every vertex in V_0 is adjacent to at least one vertex in V_2 and the subgraph induced by $V_1 \cup V_2$ has no isolated vertex. The weight of f is $\omega(f) = \sum_{v \in V(G)} f(v)$. The minimum weight among all total Roman dominating functions on G is the total Roman domination number of G , denoted by $\gamma_{tR}(G)$. It is known that the general problem of computing $\gamma_{tR}(G)$ is NP-hard. In this paper, we show that if G is a graph with no isolated vertex and H is a nontrivial graph, then the total Roman domination number of the lexicographic product graph $G \circ H$ is given by

$$\gamma_{tR}(G \circ H) = \begin{cases} 2\gamma_t(G) & \text{if } \gamma(H) \geq 2, \\ \xi(G) & \text{if } \gamma(H) = 1, \end{cases}$$

where $\gamma(H)$ is the domination number of H , $\gamma_t(G)$ is the total domination number of G and $\xi(G)$ is a domination parameter defined on G .

Keywords: Total Roman domination, total domination, lexicographic product graph.

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1 Introduction

Let G be a graph with no isolated vertex and $f: V(G) \rightarrow \{0, 1, 2\}$ a function. Let $V_i = \{x \in V(G) : f(x) = i\}$ for every $i \in \{0, 1, 2\}$. We will identify f with the partition of

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$V(G)$ induced by f and write $f(V_0, V_1, V_2)$. The weight of f is defined to be

$$\omega(f) = f(V(G)) = \sum_{v \in V(G)} f(v) = |V_1| + 2|V_2|.$$

A function $f(V_0, V_1, V_2)$ is said to be *total Roman dominating function* on G if every vertex in V_0 is adjacent to at least one vertex in V_2 and the subgraph induced by $V_1 \cup V_2$ has no isolated vertex [17]. The minimum weight among all total Roman dominating functions on G is the *total Roman domination number* of G , denoted by $\gamma_{tR}(G)$. In this article, we continue the study initiated in [5] on the total Roman domination number of lexicographic product graphs. In particular, we give closed formulas for the total Roman domination number of lexicographic product graphs.

Let G and H be two graphs. The *lexicographic product* of G and H is the graph $G \circ H$ whose vertex set is $V(G \circ H) = V(G) \times V(H)$ and $(u, v)(x, y) \in E(G \circ H)$ if and only if $ux \in E(G)$ or $u = x$ and $vy \in E(H)$. Notice that for any $u \in V(G)$ the subgraph of $G \circ H$ induced by $\{u\} \times V(H)$ is isomorphic to H . For simplicity, we will denote this subgraph by H_u .

For a basic introduction to the lexicographic product of two graphs we suggest the books [7, 12]. One of the main problems in the study of $G \circ H$ consists of finding exact values or tight bounds for specific parameters of these graphs and express them in terms of known invariants of G and H . In particular, we cite the following works on domination theory of lexicographic product graphs: (total) domination [14, 18, 19, 21], Roman domination [14], weak Roman domination [20], rainbow domination [15], super domination [6], doubly connected domination [2], secure domination [13], double domination [3] and total Roman domination [5].

We assume that the reader is familiar with the basic concepts and terminology of domination in graph. If this is not the case, we suggest the textbooks [8, 9, 11]. In particular, we use the standard notation $\gamma(G)$ and $\gamma_t(G)$ for the domination number and the total domination number of a graph G , respectively. Throughout the paper, $N(v)$ will denote the set of neighbours or *open neighbourhood* of v in G . The *closed neighbourhood* of v , denoted by $N[v]$, equals $N(v) \cup \{v\}$. A vertex $v \in V(G)$ such that $N[v] = V(G)$ is said to be a *universal vertex*. For the remainder of the paper, definitions will be introduced whenever a concept is needed.

2 The case where $\gamma(H) \geq 2$

The next theorem merges two results obtained in [14] and [21].

Theorem 2.1 ([14] and [21]). *For any graph G with no isolated vertex and any nontrivial graph H ,*

$$\gamma(G \circ H) = \begin{cases} \gamma(G), & \text{if } \gamma(H) = 1, \\ \gamma_t(G), & \text{if } \gamma(H) \geq 2. \end{cases}$$

Below we present two theorems that complete the tools we need to deduce our first result.

Theorem 2.2 ([1]). *For any graph G with no isolated vertex,*

$$2\gamma(G) \leq \gamma_{tR}(G) \leq \min\{2\gamma_t(G), 3\gamma(G)\}.$$

Theorem 2.3 ([4]). *For any graph G with no isolated vertex and any nontrivial graph H ,*

$$\gamma_t(G \circ H) = \gamma_t(G).$$

From the results above we deduce the following main theorem.

Theorem 2.4. *For any graph G with no isolated vertex and any graph H with $\gamma(H) \geq 2$,*

$$\gamma_{tR}(G \circ H) = 2\gamma_t(G).$$

Proof. The result immediately follows by applying Theorems 2.1, 2.3 and 2.2, in this order, i.e., $2\gamma_t(G) = 2\gamma(G \circ H) \leq \gamma_{tR}(G \circ H) \leq 2\gamma_t(G \circ H) = 2\gamma_t(G)$. \square

Notice that, since the general optimization problem of finding the total domination number of a graph is NP-hard [16], by Theorem 2.4 we can conclude that the problem of finding the total Roman domination number is NP-hard. Even so, we would like to point out that there are several families of graphs for which the total domination number can be found in polynomial time [10].

3 The case where $\gamma(H) = 1$

The following two lemmas are the main tools in this section.

Lemma 3.1. *Let G be a graph with no isolated vertex. For any nontrivial graph H with $\gamma(H) = 1$, there exists a $\gamma_{tR}(G \circ H)$ -function f satisfying the following two conditions.*

- (i) $f(V(H_u)) \leq 2$ for every $u \in V(G)$.
- (ii) If $f(V(H_u)) = 2$, then $f(u, v) = 2$ for some universal vertex v of H .

Proof. Given a TRDF f on $G \circ H$, we define the set $R_f = \{x \in V(G) : f(V(H_x)) \geq 3\}$. Let f be a $\gamma_{tR}(G \circ H)$ -function such that $|R_f|$ is minimum among all $\gamma_{tR}(G \circ H)$ -functions. Let $v \in V(H)$ be a universal vertex and suppose that there exists $u \in R_f$. We differentiate the following two cases.

Case 1. There exists $u' \in N(u)$ such that $f(V(H_{u'})) \geq 1$. Let f' be the function defined by $f'(V(H_u)) = f'(u, v) = 2$ and $f'(x, y) = f(x, y)$ for every $x \in V(G) \setminus \{u\}$. It is readily seen that f' is a $\gamma_{tR}(G \circ H)$ -function with $|R_{f'}| < |R_f|$, which is a contradiction.

Case 2. $f(N(u) \times V(H)) = 0$. In this case, we choose a vertex $u' \in N(u)$ and define a function f' as $f'(V(H_{u'})) = f'(u', v) = 1$, $f'(V(H_u)) = f'(u, v) = 2$ and $f'(x, y) = f(x, y)$ for every $x \in V(G) \setminus \{u, u'\}$. As in Case 1, f' is a $\gamma_{tR}(G \circ H)$ -function with $|R_{f'}| < |R_f|$, which is a contradiction.

According to the two cases above, (i) follows. Now, for any $\gamma_{tR}(G \circ H)$ -function $f(V_0, V_1, V_2)$ satisfying (i), we define $R'_f = \{x \in V(G) : f(V(H_x)) = 2 \text{ and } V(H_x) \cap V_2 = \emptyset\}$. Let $g(V'_0, V'_1, V'_2)$ be a $\gamma_{tR}(G \circ H)$ -function such that $|R'_g|$ is minimum among all $\gamma_{tR}(G \circ H)$ -functions satisfying (i). Suppose that there exists $u \in R'_g$. If there exists $u' \in N(u)$ such that, $g(V(H_{u'})) = 2$, then the function g' defined by $g'(V(H_u)) = g'(u, v) = 1$ and $g'(x, y) = g(x, y)$ for every $x \in V(G) \setminus \{u\}$, is a TRDF on $G \circ H$ of weight $\omega(g') < \omega(g) = \gamma_{tR}(G \circ H)$, which is a contradiction. Hence, $g(N(u) \times V(H)) \leq 1$ and we can differentiate the following two cases.

Case 1'. There exists $u' \in N(u)$ such that $g(V(H_{u'})) = 1$. In this case, we define a function g' by $g'(V(H_u)) = g'(u, v) = 2$ and $g'(x, y) = g(x, y)$ for every $x \in V(G) \setminus \{u\}$. Notice that g' is a $\gamma_{tR}(G \circ H)$ -function satisfying (i) and $|R'_{g'}| < |R'_g|$, which is a contradiction.

Case 2'. $g(N(u) \times V(H)) = 0$. We fix $u' \in N(u)$. Notice that there exists $u'' \in N(u') \setminus \{u\}$, with $V(H_{u''}) \cap V'_2 \neq \emptyset$. Hence, we can define a function g' as $g'(V(H_{u'})) = g'(u', v) = g'(V(H_u)) = g'(u, v) = 1$ and $g'(x, y) = g(x, y)$ for every $x \in V(G) \setminus \{u, u'\}$. As in Case 1', g' is a $\gamma_{tR}(G \circ H)$ -function satisfying (i) and $|R'_{g'}| < |R'_g|$, which is a contradiction.

According to the two cases above, $R'_g = \emptyset$, and so there exists a $\gamma_{tR}(G \circ H)$ -function h defined as $h(V(H_u)) = h(u, v) = 2$ whenever $g(V(H_u)) = 2$ and $h(V(H_u)) = g(V(H_u))$ otherwise. Therefore, h satisfies (i) and (ii). \square

Lemma 3.2. *Let G be a graph with no isolated vertex and H a nontrivial graph with $\gamma(H) = 1$. Let $f(V_0, V_1, V_2)$ be a $\gamma_{tR}(G \circ H)$ -function, $A = \{x \in V(G) : V(H_x) \cap V_1 \neq \emptyset\}$ and $B = \{x \in V(G) : V(H_x) \cap V_2 \neq \emptyset\}$. If f satisfies Lemma 3.1, then B is a dominating set and $A \cup B$ is a total dominating set of G .*

Proof. Let $f(V_0, V_1, V_2)$ be a $\gamma_{tR}(G \circ H)$ -function which satisfies Lemma 3.1. Let $C = V(G) \setminus (A \cup B)$. Obviously, if $x \in C$, then $V(H_x) \subseteq V_0$, which implies that x is adjacent to some vertex in B and, since H is a nontrivial graph and f satisfies Lemma 3.1, if $x \in A$, then there exists $y \in V(H)$ such that $(x, y) \in V_0$, and so x is adjacent to some vertex in B . Hence, B is a dominating set of G . Now, since the subgraph of $G \circ H$ induced by $V_1 \cup V_2$ does not have isolated vertices, the subgraph of G induced by $A \cup B$ does not have isolated vertices, which implies that $A \cup B$ is total dominating set of G . \square

For any graph G , let $\mathcal{D}(G)$ be the set of dominating sets of G , and $\mathcal{D}_t(G)$ the set of total dominating sets of G . We now proceed to introduce our main tool, which is the following domination parameter.

$$\xi(G) = \min\{|A| + 2|B| : B \in \mathcal{D}(G) \text{ and } A \cup B \in \mathcal{D}_t(G)\}.$$

We say that an ordered pair (A, B) of subsets of $V(G)$ is a $\xi(G)$ -pair if $B \in \mathcal{D}(G)$, $A \cup B \in \mathcal{D}_t(G)$ and $\xi(G) = |A| + 2|B|$.

Theorem 3.3. *For any graph G with no isolated vertex and any nontrivial graph H with $\gamma(H) = 1$,*

$$\gamma_{tR}(G \circ H) = \xi(G).$$

Proof. Let v be a universal vertex of H . From any $\xi(G)$ -pair (A, B) we define the function $f(V_0, V_1, V_2)$ as $V_2 = B \times \{v\}$, $V_1 = A \times \{v\}$ and $V_0 = V(G \circ H) \setminus (V_1 \cup V_2)$. Since V_2 is a dominating set of $G \circ H$ and $V_1 \cup V_2$ is a total dominating set of $G \circ H$, we can conclude that f is a TRDF on $G \circ H$. Therefore, $\gamma_{tR}(G \circ H) \leq \omega(f) = |V_1| + 2|V_2| = |A| + 2|B| = \xi(G)$.

Now, let $f'(V'_0, V'_1, V'_2)$ be a $\gamma_{tR}(G \circ H)$ -function which satisfies Lemma 3.1. Let $A = \{x \in V(G) : f'(V(H_x)) = 1\}$ and $B = \{x \in V(G) : f'(V(H_x)) = 2\}$. By Lemma 3.2, B is a dominating set of G and $A \cup B$ is a total dominating set, which implies that $\xi(G) \leq |A| + 2|B| = |V'_1| + 2|V'_2| = \gamma_{tR}(G \circ H)$. Therefore, the result follows. \square

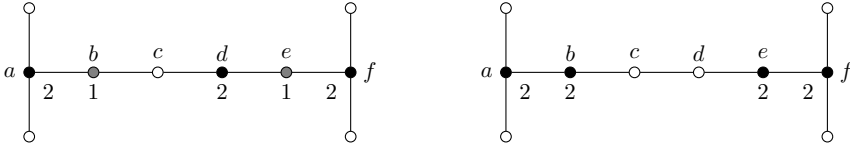


Figure 1: The labels correspond to two different $\gamma_{tR}(G)$ -functions $f_1(V_0, V_1, V_2)$, on the left, and $f_2(W_0, W_1, W_2)$, on the right. In this case, $\gamma_{tR}(G) = 2\gamma_t(G) = 8$, $V_2 = \{a, d, f\}$ is a $\gamma(G)$ -set and $W_2 = \{a, b, e, f\}$ is the only $\gamma_t(G)$ -set.

Let G be the graph shown in Figure 1 and H a nontrivial graph with $\gamma(H) = 1$. Notice that $\gamma_{tR}(G \circ H) = \xi(G) = \gamma_{tR}(G) = 8$, where $f_1(V_0, V_1, V_2)$ and $f_2(W_0, W_1, W_2)$ are $\gamma_{tR}(G)$ -functions for $V_1 = \{b, e\}$, $V_2 = \{a, d, f\}$, $W_1 = \emptyset$, $W_2 = \{a, b, e, f\}$. Furthermore, both (V_1, V_2) and (W_1, W_2) are $\xi(G)$ -pairs, where V_2 is a $\gamma(G)$ -set and $|V_1| + |V_2| > \gamma_t(G)$, while W_2 is a $\gamma_t(G)$ -set which does not contain any $\gamma(G)$ -set.

The following bounds were given in [5]. In fact the lower bound was stated for any connected non-trivial graph G , although it also holds for any graph G with no isolated vertex.

Theorem 3.4 ([5]). *For any graph H and any graph G with no isolated vertex,*

$$\gamma_{tR}(G) \leq \gamma_{tR}(G \circ H) \leq 2\gamma_t(G).$$

Furthermore, if $\gamma(H) = 1$, then

$$\gamma_{tR}(G \circ H) \leq 3\gamma(G).$$

In order to improve some of these bounds, we need to introduce some additional terminology. Given a set $S \subseteq V(G)$, we define

$$\psi(S) = \min\{|S'| : S' \subseteq V(G) \setminus S \text{ and } S \subseteq N(S' \cup S)\}.$$

We also define the following parameter associated to G .

$$\mu(G) = \min\{\psi(S) : S \text{ is a } \gamma(G)\text{-set}\}.$$

It is readily seen that $0 \leq \mu(G) \leq \gamma(G)$. Furthermore, $\mu(G) = 0$ if and only if $\gamma_t(G) = \gamma(G)$, while $\mu(G) = \gamma(G)$ if and only if for every $\gamma(G)$ -set S and every pair of different vertices $x, y \in S$ we have that $N[x] \cap N[y] = \emptyset$, i.e., if and only if every $\gamma(G)$ -set is a 2-packing of G .

With the notation above in mind, we state the following theorem.

Theorem 3.5. *Let G and H be two graphs with no isolated vertex. If $\gamma(H) = 1$, then*

$$\max\{\gamma_{tR}(G), \gamma_t(G) + \gamma(G)\} \leq \gamma_{tR}(G \circ H) \leq \min\{2\gamma(G) + \mu(G), 2\gamma_t(G)\}.$$

Proof. Our main tool is Theorem 3.3. For any $\xi(G)$ -pair (A, B) we have that $\gamma_{tR}(G \circ H) = \xi(G) = 2|B| + |A| \geq |(A \cup B)| + |B| \geq \gamma_t(G) + \gamma(G)$.

Now, let S be a $\gamma(G)$ -set with $\mu(G) = \psi(S)$ and $S' \subseteq V(G) \setminus S$ a set of minimum cardinality among the subsets of $V(G) \setminus S$ satisfying that $S \subseteq N(S' \cup S)$. Since $S \cup S'$ is a total dominating set, $\gamma_{tR}(G \circ H) = \xi(G) \leq |S \cup S'| + |S| = 2|S| + |S'| = 2\gamma(G) + \mu(G)$.

Finally, by Theorem 3.4, $\gamma_{tR}(G) \leq \gamma_{tR}(G \circ H) \leq 2\gamma_t(G)$, which completes the proof. \square

Since $\mu(G) \leq \gamma(G)$, we can conclude that the bound $\gamma_{tR}(G \circ H) \leq 2\gamma(G) + \mu(G)$ is never worse than the known bound $\gamma_{tR}(G \circ H) \leq 3\gamma(G)$. In order to see that the upper bounds given by Theorem 3.5 are tight, we take the graph G shown in Figure 1 and any nontrivial graph H with $\gamma(H) = 1$. In this case, $\gamma_{tR}(G \circ H) = 2\gamma_t(G) = 2\gamma(G) + \mu(G) = 8$.

We would point out the following result which is a direct consequence of Theorems 2.2 and 3.5.

Theorem 3.6. *If G is a graph with $\gamma_t(G) = \gamma(G)$ and H is a nontrivial graph with $\gamma(H) = 1$, then*

$$\gamma_{tR}(G \circ H) = \gamma_{tR}(G) = 2\gamma(G).$$

We now proceed to characterize the graphs achieving the lower bounds given by Theorem 3.5.

Theorem 3.7. *Let G and H be two graphs with no isolated vertex. If $\gamma(H) = 1$, then the following statements are equivalent.*

- (i) $\gamma_{tR}(G \circ H) = \gamma_{tR}(G)$.
- (ii) *There exists a $\gamma_{tR}(G)$ -function $f(V_0, V_1, V_2)$ such that V_2 is dominating set of G .*

Proof. If there exists a $\gamma_{tR}(G)$ -function $f(V_0, V_1, V_2)$ such that V_2 is dominating set of G , then $\gamma_{tR}(G \circ H) = \xi(G) \leq |V_1 \cup V_2| + |V_2| = |V_1| + 2|V_2| = \gamma_{tR}(G)$. Since $\gamma_{tR}(G) \leq \gamma_{tR}(G \circ H)$, we conclude that $\gamma_{tR}(G \circ H) = \gamma_{tR}(G)$.

Conversely, assume that $\gamma_{tR}(G \circ H) = \gamma_{tR}(G)$. Let $g(V'_0, V'_1, V'_2)$ be a $\gamma_{tR}(G \circ H)$ -function satisfying Lemma 3.1. Let $A = \{x \in V(G) : g(V(H_x)) = 1\}$ and $B = \{x \in V(G) : g(V(H_x)) = 2\}$. By Lemma 3.2, B is a dominating set of G and $A \cup B$ is a total dominating set. Hence, we can define a TRDF $h(V''_0, V''_1, V''_2)$ from $V''_1 = A$ and $V''_2 = B$. Since $\omega(h) = |A| + 2|B| = |V'_1| + 2|V'_2| = \gamma_{tR}(G \circ H) = \gamma_{tR}(G)$, we conclude that h is a $\gamma_{tR}(G)$ -function where V''_2 is a dominating set, as desired. \square

The next result gives a characterization for the case $\gamma_{tR}(G \circ H) = \gamma_t(G) + \gamma(G)$ whenever $\gamma(H) = 1$.

Theorem 3.8. *Let G and H be two graphs with no isolated vertex. If $\gamma(H) = 1$, then the following statement are equivalent.*

- (i) $\gamma_{tR}(G \circ H) = \gamma_t(G) + \gamma(G)$.
- (ii) *There exists a $\gamma_t(G)$ -set that contains some $\gamma(G)$ -set.*

Proof. If there exists a $\gamma_t(G)$ -set X which contains a $\gamma(G)$ -set B , then $\gamma_{tR}(G \circ H) = \xi(G) \leq |X \setminus B| + 2|B| = |X| + |B| = \gamma_t(G) + \gamma(G)$, and by (i) we conclude that $\gamma_{tR}(G \circ H) = \gamma_t(G) + \gamma(G)$.

Conversely, assume that $\gamma_{tR}(G \circ H) = \gamma_t(G) + \gamma(G)$ and let (A, B) be a $\xi(G)$ -pair. If the total dominating set $A \cup B$ is a $\gamma_t(G)$ -set, then we are done, as B is a dominating set and from $\gamma_t(G) + \gamma(G) = \gamma_{tR}(G \circ H) = \xi(G) = |A| + 2|B| = |A \cup B| + |B| = \gamma_t(G) + |B|$ we deduce that B is a $\gamma(G)$ -set. Suppose to the contrary, that $|A \cup B| > \gamma_t(G)$. In such a case, $\gamma_t(G) + \gamma(G) = \xi(G) = |A| + 2|B| \geq |A \cup B| + |B| > \gamma_t(G) + \gamma(G)$, which is a contradiction. Therefore, the result follows. \square

Figure 2 shows a graph G such that $\gamma_{tR}(G \circ H) = \gamma_t(G) + \gamma(G) = 7 > 6 = \gamma_{tR}(G)$ for every nontrivial graph H with $\gamma(H) = 1$.

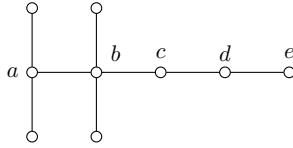


Figure 2: The $\gamma_t(G)$ -set $D = \{a, b, d, e\}$ contains the $\gamma(G)$ -set $S = \{a, b, d\}$.

4 Small values of $\gamma_{tR}(G \circ H)$

In this short section we characterize the graphs G and H for which $\gamma_{tR}(G \circ H) \in \{3, 4\}$.

Theorem 4.1. *For any graph G and H with no isolated vertex, the following statements are equivalent.*

- (i) $\gamma_{tR}(G \circ H) = 3$.
- (ii) $\gamma(G) = \gamma(H) = 1$.

Proof. If $\gamma_{tR}(G \circ H) = 3$, then by Theorem 2.4 we deduce that $\gamma(H) = 1$. Moreover, by Theorem 3.5 we have that $3 = \gamma_{tR}(G \circ H) \geq \gamma_t(G) + \gamma(G) \geq 3$. Hence, $\gamma(G) = 1$, as required. Conversely, if $\gamma(G) = \gamma(H) = 1$, then by Theorem 3.8 we deduce that $\gamma_{tR}(G \circ H) = 3$. □

Theorem 4.2. *For any graph G and H with no isolated vertex, $\gamma_{tR}(G \circ H) = 4$ if and only if one of the following conditions are satisfied.*

- (i) $\gamma_t(G) = 2$ and $\gamma(H) \geq 2$.
- (ii) $\gamma_t(G) = \gamma(G) = 2$ and $\gamma(H) = 1$.

Proof. We first notice that if conditions (i) or (ii) holds, then by Theorem 2.4 or by Theorem 3.5, respectively, it follows that $\gamma_{tR}(G \circ H) = 4$.

Conversely, assume that $\gamma_{tR}(G \circ H) = 4$. If $\gamma(H) \geq 2$, then Theorem 2.4 leads to $\gamma_t(G) = 2$. From now on, we assume that $\gamma(H) = 1$. By Theorem 3.8, we have that $4 = \gamma_{tR}(G \circ H) \geq \gamma_t(G) + \gamma(G)$. Hence, $1 \leq \gamma(G) \leq 2$. If $\gamma(G) = 1$, then by Theorem 4.1 we obtain that $\gamma_{tR}(G \circ H) = 3$, which is a contradiction. Hence, $\gamma(G) = 2$ and so $\gamma_t(G) = 2$. Therefore, the result follows. □

5 Open problems

By Theorem 3.3 we learned that, if we want to know the behaviour of $\gamma_{tR}(G \circ H)$ when $\gamma(H) = 1$, then it is crucial to obtain the exact value or derive tight bounds on $\xi(G)$. In this sense, the study of $\xi(G)$ is an interesting challenge.

In particular, Theorem 3.5 states that

$$\max\{\gamma_{tR}(G), \gamma_t(G) + \gamma(G)\} \leq \xi(G) \leq \min\{2\gamma(G) + \mu(G), 2\gamma_t(G)\}.$$

The graphs achieving the equalities $\xi(G) = \gamma_{tR}(G)$ and $\xi(G) = \gamma_t(G) + \gamma(G)$ were characterized in Theorems 3.7 and 3.8, respectively. Therefore, the problems of characterizing the graphs achieving the equalities $\xi(G) = 2\gamma_t(G)$ and $\xi(G) = 2\gamma(G) + \mu(G) = 3\gamma(G)$ remain open.

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Wiener-type indices of Parikh word representable graphs*

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Abstract

A new class of graphs $G(w)$, called Parikh word representable graphs (*PWRG*), corresponding to words w that are finite sequence of symbols, was considered in the recent past. Several properties of these graphs have been established. In this paper, we consider these graphs corresponding to binary core words of the form aub over a binary alphabet $\{a, b\}$. We derive formulas for computing the Wiener index of the *PWRG* of a binary core word. Sharp bounds are established on the value of this index in terms of different parameters related to binary words over $\{a, b\}$ and the corresponding *PWRGs*. Certain other Wiener-type indices that are variants of Wiener index are also considered. Formulas for computing these indices in the case of *PWRG* of a binary core word are obtained.

Keywords: Graphs, words, Parikh matrix, Parikh word representable graphs.

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1 Introduction

While words that are finite sequences of symbols are the fundamental and central objects in computing models developed in theoretical studies of computer science, graphs are mathematical models of pairwise relations between objects found useful for analyzing and solving different kinds of problems. An interesting area of investigation is relating graphs and words and there are many studies in this direction (see, for example, [7, 10, 15, 18, 19, 24]).

On the other hand, in the study of numerical quantities related to subwords (also called scattered subwords) of a word, the notion of Parikh matrix of a word over an ordered alphabet was introduced in [26]. This has opened up a new direction of research in the area of combinatorics on words [23] and many problems on words and subwords have been investigated (see, for example, [1, 2, 4, 25, 33, 34, 36, 37, 38] and references therein), resulting in a number of interesting results. Parikh word representable graph (*PWRG*) is one such notion introduced in [3] linking the two areas of study on properties of words and of graphs. Based on the notions of subwords of a word and the Parikh matrix of a word [26] with entries of the matrix giving the counts of certain subwords in the word, *PWRG* related to a word was introduced in [3]. Relationship of these graphs with corresponding words and partitions was recently studied in [27].

In the field of chemical graph theory [14], undirected graphs, referred to as molecular graphs are considered providing graph representations of organic compounds or equivalently their molecular structures with atoms other than hydrogen often represented by vertices and covalent chemical bonds by edges. In fact in chemical graph theory there have been attempts to capture the molecular structure in terms of the topological index of the corresponding graph. There has been a great interest in various topological indices associated with graphs due to their application in the area of chemical graph theory [8]. There are a number of studies (see, for example, [14]) of various topological indices of graphs establishing formulae for computing the indices and also providing upper and lower bounds on the values of such indices. The Wiener index (also called Wiener number) [40] is the first topological index introduced by Harold Wiener. Knor et al. [22] provide an excellent summary of results relating to Wiener index besides providing conjectures and problems on this index. Wiener index and its variants for different classes of graphs are widely investigated indices (see, for example, [9, 12, 14, 21, 28, 29, 39] and references therein).

In this paper we study the Wiener index of a *PWRG* of a binary core word and derive formulas for computing this index besides establishing sharp bounds on their values, given different parameters related to the graphs. We also obtain formulas for evaluating certain other indices that are variants of Wiener index, such as multiplicative Wiener index [13], terminal Wiener index [11], peripheral Wiener index [16], hyper-Wiener index [20, 30] in the case of a *PWRG* of a binary core word.

2 Preliminaries

The basic notions and notations relating to words and subwords can be found in [23, 31]. We recall some essential concepts and results. An ordered alphabet Σ which is a set of symbols $\{a_1, a_2, \dots, a_s\}$ with an ordering $<$ on its symbols is written as $\Sigma = \{a_1 < a_2 < \dots < a_s\}$. A word v is a subword of a word w over Σ if and only if we can find words $x_1, x_2, \dots, x_n, y_0, y_1, \dots, y_n$ over Σ , some of them possibly empty, such that $w = y_0x_1y_1x_2y_2 \dots y_{n-1}x_ny_n$ and $v = x_1x_2 \dots x_n$. The number of occurrences of a word u as a subword of w is denoted by $|w|_u$. For example, in the word $w = aababaaab =$

a^2baba^3b over the ordered binary alphabet $\Sigma = \{a < b\}$, the number of distinct occurrences of the subword ab is 11 so that $|w|_{ab} = 11$. The set of all words over an alphabet Σ , including the empty word λ with no symbols, is denoted by Σ^* .

Definition 2.1 ([6]). A binary word w over an alphabet $\{a, b\}$ is said to be fair if $|w|_{ab} = |w|_{ba}$.

Example 2.2. The binary word $abbbaab$ is a fair word since $|w|_{ab} = |w|_{ba} = 6$.

Definition 2.3 ([38]). Consider the binary word $w \in \Sigma^*$ where $\Sigma = \{a < b\}$. The core of w , denoted by $\text{core}(w)$, is the unique word w_0 of w with the smallest possible length such that $w \in b^*w_0a^*$. A word $w \in \Sigma^*$ is said to be a core word if and only if $\text{core}(w) = w$.

Clearly, a non empty word w over $\Sigma = \{a < b\}$ is a core word if and only if w starts with a and ends with b .

We now recall the relationship between binary core words and partitions following the discussion in [38, pages 62–63].

Lemma 2.4 ([38]). *Every nonempty binary core word can be identified with a partition of a positive integer.*

Proof. Suppose $w \in \Sigma^*$ is a nonempty core word and has the form $a^{n_1}ba^{n_2}b \dots a^{n_{|w|_b}}b$ where $n_1 \geq 1$ and n_k is nonnegative for each $k, 2 \leq k \leq |w|_b$. Thus w can be identified with the partition

$$|w|_{ab} = (n_1 + n_2 + \dots + n_{|w|_b}) + \dots + (n_2 + n_1) + n_1.$$

Clearly, distinct core words are identified with distinct partitions.

Conversely, suppose that $m_1 + m_2 + \dots + m_l$ is a partition of some positive integer, where $m_1 \geq m_2 \geq \dots \geq m_l \geq 1$. It is clear that the word

$$w = a^{m_1}ba^{m_1-1-m_l}ba^{m_1-2-m_l-1}b \dots a^{m_1-m_2}b$$

can be identified with the given partition. □

We shall use the notation $p(w) = (n_1 + n_2 + \dots + n_l) + (n_1 + n_2 + \dots + n_{l-1}) + \dots + (n_1 + n_2 + \dots + n_{l-i+1}) + \dots + (n_1 + n_2) + (n_1)$ to indicate the partition corresponding to the word $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b$.

We now recall the notion of Parikh word representable graph (PWVG) [3]. For basic concepts pertaining to graphs we refer to [5].

Definition 2.5 ([3]). For a word $w = a_1a_2 \dots a_n$ of length n where for $1 \leq i \leq n$, $a_i \in \Sigma = \{a < b\}$, we associate a simple graph $G = G(w)$ with n vertices $\{1, 2, \dots, n\}$. Each vertex i has the label a_i and represents the position of the letter $a_i, 1 \leq i \leq n$, in w . For each occurrence of the subword ab in w , there is an edge in $G(w)$ joining the vertices corresponding to the positions of a and b in w . We say that the graph G is Parikh binary word representable by the binary word w . In other words, we say that a graph G is *Parikh binary word representable* if there exists a binary word w such that G is Parikh binary word representable by the binary word w .

Since every connected Parikh binary word representable graph corresponds to a core word, we deal with only core words and the corresponding graphs in the rest of this paper. As an illustration, if the core word is $w = aabab$, then in the Parikh word representable graph as shown in Figure 1, the vertices 1, 2 and 4 have label a while the vertices 3 and 5 have the label b . The number of edges in the graph is $|w|_{ab} = 5$. For example there is a subword ab in w formed by the symbol a in position 1 and the symbol b in position 3 and so in the graph there is an edge joining the vertex 1 with the vertex 3.

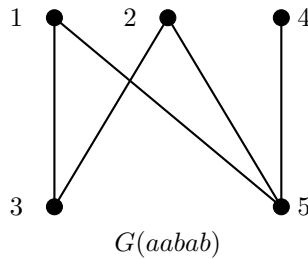


Figure 1: The Parikh word representable graph of the word $aabab$.

3 Wiener index of Parikh word representable graphs

Let $G = (V, E)$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The distance between the vertices u and v of G is denoted by $d(u, v)$ and is defined as the length of a shortest path between u and v in G .

Definition 3.1. The Wiener index $W(G)$ of a connected graph $G = (V, E)$, is the sum of distances $d(u, v)$ between all the vertices u and v of G . In other words

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v).$$

We now obtain a formula for computing the Wiener index of Parikh word representable graph of a binary word.

Theorem 3.2. The Wiener index of a Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b$, $n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is

$$W(G(w)) = \left(\sum_{i=1}^l n_i \right)^2 + \sum_{i=1}^l (l + 2i - 3)n_i + l(l - 1).$$

Proof. In the Parikh word representable graph $G(w)$ corresponding to the word $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b$, we consider pairs of vertices (u, v) , with $u, v \in \{1, 2, \dots, n\}$ where the label of u appears before the label of v in w . There are now four cases to be considered:

- (i) u and v are both labeled a ;
- (ii) u is labeled a and v is labeled b ;
- (iii) u is labeled b and v is labeled a ;

(iv) u and v are both labeled b .

The contribution to the Wiener index of the Parikh word representable graph from each of these four cases may be calculated as follows:

(i) The distance between any two vertices labeled a is 2 and there are $n_1 + n_2 + \dots + n_l$ vertices labeled a . Hence the total contribution from these pairs of vertices is

$$(n_1 + n_2 + \dots + n_l)C_2 \times 2 = (n_1 + n_2 + \dots + n_l)^2 - (n_1 + n_2 + \dots + n_l).$$

(ii) The distance between u labeled a and v labeled b is 1 and there are $n_1 + (n_1 + n_2) + \dots + (n_1 + n_2 + \dots + n_l)$ such pairs. Hence the total contribution is

$$n_1 + (n_1 + n_2) + \dots + (n_1 + n_2 + \dots + n_l) = ln_1 + (l - 1)n_2 + \dots + n_l.$$

(iii) The distance between u labeled b and v labeled a is 3 and there are $(n_2 + n_3 + \dots + n_l) + (n_3 + \dots + n_l) + \dots + n_l = n_2 + 2n_3 + \dots + (l - 1)n_l$ such pairs. Hence the total contribution is

$$3(n_2 + 2n_3 + \dots + (l - 1)n_l).$$

(iv) The distance between any two vertices labeled b is 2 and there are l vertices labeled b . Hence the total contribution from these pairs of vertices is

$$lC_2 \times 2 = l(l - 1).$$

Hence the Wiener index of $G(w)$ is given by

$$\begin{aligned} W(G(w)) &= (n_1 + n_2 + \dots + n_l)^2 + (l - 1)n_1 + (l + 1)n_2 + \dots \\ &\quad + 3(l - 1)n_l + l(l - 1) \\ &= \left(\sum_{i=1}^l n_i \right)^2 + \sum_{i=1}^l (l + 2i - 3)n_i + l(l - 1). \end{aligned} \quad \square$$

Example 3.3. For the PWRG in Figure 1 corresponding to the word $w = a^2bab$, we have $l = 2, n_1 = 2, n_2 = 1$ and so $W(G(w)) = 16$ which can also be verified from the formula in the Definition 3.1 by actually computing the distances $d(u, v)$ for all unordered pairs (u, v) of vertices.

We now derive an alternate form of the expression for the Wiener index of the Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$. An interesting aspect of this alternate form is that the expression in the formula is elegant involving only the parameters related to the word.

Theorem 3.4. *The Wiener index of a Parikh word representable graph $G(w)$, for $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is*

$$W(G(w)) = |w|^2 - |w| + |w|_a|w|_b - 2|w|_{ab}.$$

Proof. Since $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, we have $\sum_{i=1}^l n_i = |w|_a, l = |w|_b$. Also

$$\begin{aligned} |w|_a|w|_b - |w|_{ab} &= l \left(\sum_{i=1}^l n_i \right) - [(n_1 + n_2 + \cdots + n_l) + \cdots + (n_1 + n_2) + n_1] \\ &= \sum_{i=1}^l in_i - |w|_a \end{aligned}$$

so that

$$\sum_{i=1}^l in_i = |w|_a|w|_b + |w|_a - |w|_{ab}.$$

Hence from Theorem 3.2, the Wiener index

$$\begin{aligned} W(G(w)) &= |w|_a^2 + (|w|_b - 3)|w|_a + |w|_b(|w|_b - 1) + 2 \sum_{i=1}^l in_i \\ &= |w|_a^2 + |w|_b^2 + 3|w|_a|w|_b - |w|_a - |w|_b - 2|w|_{ab} \\ &= |w|^2 - |w| + |w|_a|w|_b - 2|w|_{ab} \end{aligned}$$

using $|w| = |w|_a + |w|_b$. □

Corollary 3.5. *The Wiener index of a Parikh word representable graph $G(w)$ for a fair word $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is*

$$W(G(w)) = |w|^2 - |w|.$$

Proof. For a binary word w , we have $|w|_{ab} + |w|_{ba} = |w|_a|w|_b$. Since w is a fair word, $|w|_{ab} = |w|_{ba}$ so that $|w|_a|w|_b - 2|w|_{ab} = |w|_{ba} - |w|_{ab} = 0$. Hence from Theorem 3.4, $W(G(w)) = |w|^2 - |w|$. □

Theorem 3.6. *The Wiener index $W(G(w))$ of a Parikh word representable graph $G(w) = (V_1 \cup V_2, E)$ with $|V_1| = |w|_a = p, |V_2| = |w|_b = q$ for the word $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is bounded above by $p^2 + q^2 + 3pq - 3p - 3q + 2$ and below by $p^2 + q^2 + pq - p - q$. The bounds are attained on $G(ab^{q-1}a^{p-1}b)$ and $G(a^pb^q)$ respectively.*

Proof. Since $G(w)$ is connected, $|w|_{ab} = |E| \geq p + q - 1$ [5]. Also $|w|_{ab} \leq pq$ [26]. Hence from Theorem 3.4, the Wiener index of $G(w)$ is

$$\begin{aligned} W(G(w)) &= p^2 + q^2 + 3pq - p - q - 2|w|_{ab} \\ &\leq p^2 + q^2 + 3pq - p - q - 2(p + q - 1) = p^2 + q^2 + 3pq - 3p - 3q + 2 \end{aligned}$$

which is the Wiener index of the Parikh word representable graph $G(ab^{q-1}a^{p-1}b)$ and

$$W(G(w)) \geq p^2 + q^2 + 3pq - p - q - 2pq = p^2 + q^2 + pq - p - q$$

which is the Wiener index of the Parikh word representable graph $G(a^pb^q)$. □

Remark 3.7. One of the conjectures listed in [22, page 333], states that for a graph G with diameter d and order $2d + 1$, the Wiener index $W(G) \leq W(C_{2d+1})$ where C_{2d+1} denotes a cycle of length $2d + 1$. Since the diameter of any *PWRG* $G(w)$ corresponding to the binary core word w is 3, this conjecture holds good for $G(w)$, if the order of $G(w)$ is 7, which also equals $|w|$. In fact, if the binary core word w with $|w| = 7$, is over the ordered alphabet $\{a < b\}$, the maximum Wiener index of $G(w)$ equals $W(C_7)$ which is 42 and this is attained, by Theorem 3.6, on $G(ab^3a^2b)$ or $G(ab^2a^3b)$.

We shall now find an expression for an upper bound on the Wiener index of Parikh word representable graph with a fixed number of edges. We use the following lemma.

Lemma 3.8. *Given a fixed value of e and of l , the maximum value of $W(G(w))$ over all Parikh word representable graphs of the form $G(w)$ for $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, with e edges, is attained on $G(ab^{l-1}a^{e-l}b)$.*

Proof. Since the number of edges in $G(w)$ is $e = |w|_{ab}, |w|_b = l$ and $e \geq |w|_a + |w|_b - 1$ as $G(w)$ is a connected graph with $|w|_a + |w|_b$ vertices, we have $|w|_a \leq e - l + 1$. Hence from Theorem 3.4, the Wiener index of $G(w)$ is

$$\begin{aligned} W(G(w)) &= |w|_a(|w|_a - 1) + l^2 + 3|w|_al - l - 2e \\ &\leq (e - l + 1)(e - l) + l^2 + 3|w|_al - l - 2e \\ &\leq (e - l + 1)(e - l) + l^2 + 3(e - l + 1)l - l - 2e = e^2 - l^2 + el + l - e \end{aligned}$$

which is the Wiener index of the Parikh word representable graph $G(ab^{l-1}a^{e-l}b)$. □

Theorem 3.9. *An upper bound of the Wiener index $W(G(w))$ of a Parikh word representable graph $G(w)$, $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, with e edges is given by*

$$W(G(w)) \leq \begin{cases} 5m^2 - 6m + 2(m \geq 1), & \text{if } e = 2m - 1; \\ 5m^2 - m(m \geq 1), & \text{if } e = 2m. \end{cases}$$

The bound is sharp and is attained on $G(ab^{m-1}a^{m-1}b)$ when $e = 2m - 1$ and on $G(ab^{m-1}a^mb)$ when $e = 2m$.

Proof. From Lemma 3.8, the Wiener index of the Parikh word representable graph $G(w)$, $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, has a maximum for $G(ab^{l-1}a^{e-l}b)$ and is given by $W(G(w)) = e^2 - l^2 + el + l - e$. We now use the fact that a quadratic expression $ax^2 + bx + c, a < 0$, has a maximum when $x = -\frac{b}{2a}$. When $e = 2m - 1, m \geq 1$, we have

$$W(G(w)) = -l^2 + 2ml + (4m^2 - 6m + 2).$$

If $e = 2m - 1$ has a fixed value, this quadratic expression in l has a maximum when $l = m$ and the maximum is $5m^2 - 6m + 2$. When $e = 2m, m \geq 1$, we have

$$W(G(w)) = -l^2 + l(1 + 2m) + (4m^2 - 2m).$$

Again if $e = 2m$ has a fixed value, this quadratic expression has a maximum when $l = [m + \frac{1}{2}] = m$ where $[x]$ is the integral part of x and the maximum is $5m^2 + 2m$. □

We shall now evaluate the Wiener index of a Parikh word representable graph corresponding to a specific partition of a given integer.

Theorem 3.10. *Suppose $m_1 + m_2 + \dots + m_l$ is a partition of some positive integer, where $m_1 \geq m_2 \geq \dots \geq m_l \geq 1$. Then the Wiener index of the Parikh word representable graph G corresponding to this partition is given by*

$$W(G) = m_1^2 - 2e + (3l - 1)m_1 + l(l - 1)$$

where e is the number of edges of G .

Proof. From Lemma 2.4, the word $w = a^{m_1}ba^{m_1-1-m_i}ba^{m_1-2-m_{i-1}}b \dots a^{m_1-m_2}b$ corresponds to the given partition. Now $|w| = m_1 + l, |w|_a = m_1, |w|_b = l$, so that using the formula in Theorem 3.4, we have

$$\begin{aligned} W(G) &= W(G(w)) = |w|^2 - |w| + |w|_a|w|_b - 2|w|_{ab} \\ &= (m_1 + l)^2 - (m_1 + l) + lm_1 - 2e = m_1^2 - 2e + (3l - 1)m_1 + l(l - 1) \end{aligned}$$

since $|w|_{ab} = e$. □

4 Multiplicative Wiener index

Definition 4.1 ([32]). The Wiener polynomial of a graph G is

$$W(G; x) = \sum_{\{u,v\} \subseteq V(G)} x^{d(u,v)}.$$

Theorem 4.2. *The Wiener polynomial of a Parikh word representable graph $G(w)$, for $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is*

$$W(G(w); x) = (|w|_a|w|_b - |w|_{ab})x^3 + \frac{1}{2}(|w|_a(|w|_a - 1) + |w|_b(|w|_b - 1))x^2 + (|w|_{ab})x.$$

Proof. We consider pairs of vertices (u, v) in the Parikh word representable graph $G(w)$ corresponding to the word $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b$, with $u, v \in \{1, 2, \dots, n\}$ where the label of u appears before the label of v in w . As discussed in the proof of Theorem 3.2, the vertex pairs are of four types, namely, types 1, 2, 3 and 4. Also, as discussed in the proof of Theorem 3.4, there are $\frac{1}{2}|w|_a(|w|_a - 1)$ pairs of vertices of type 1 and $\frac{1}{2}|w|_b(|w|_b - 1)$ of type 4 and the distance between each such pair is 2. Likewise, there are $|w|_{ab}$ pairs of vertices of type 2 with distance 1 and $|w|_a|w|_b - |w|_{ab}$ pairs of vertices of type 3 with distance 3. Hence the Wiener polynomial is

$$(|w|_a|w|_b - |w|_{ab})x^3 + \frac{1}{2}(|w|_a(|w|_a - 1) + |w|_b(|w|_b - 1))x^2 + (s|w|_{ab})x. \quad \square$$

Definition 4.3 ([40]). The Wiener polarity index of G , denoted by $W_p(G)$, is defined as $W_p(G) = |\{(u, v) \subseteq V(G) : d(u, v) = 3\}|$.

Theorem 4.4. *The Wiener polarity index of a Parikh word representable graph $G(w)$, for $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is given by*

$$W_p(G(w)) = |w|_a|w|_b - |w|_{ab}.$$

Proof. In the Parikh word representable graph $G(w)$, for the word $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$ as in the hypothesis, the pairs of vertices (u, v) of type 3 as mentioned in the proof of Theorem 4.2, are at a distance 3 and these pairs contribute to the Wiener polarity index of $G(w)$. In fact there are $n_2 + n_3 + \cdots + n_l$ vertices with label a that are at distance 3 from the vertex with label, the first b in w . Likewise for other vertices corresponding to the other b 's in w . Hence

$$\begin{aligned} W_p(G(w)) &= (n_2 + n_3 + \cdots + n_l) + (n_3 + n_4 + \cdots + n_l) + \cdots + n_l \\ &= \sum_{i=1}^l i n_i - \sum_{i=1}^l n_i = |w|_a |w|_b - |w|_{ab}. \end{aligned} \quad \square$$

Definition 4.5 ([13]). The multiplicative version of the Wiener index of a graph G is

$$\pi(G) = \prod_{\{u,v\} \subseteq V(G)} d(u, v).$$

Theorem 4.6. *The multiplicative Wiener index of a Parikh word representable graph $G(w)$, for $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is*

$$\pi(G(w)) = 2^{\frac{|w|_a(|w|_a-1)+|w|_b(|w|_b-1)}{2}} 3^{|w|_a|w|_b-|w|_{ab}}.$$

Proof. Considering pairs of vertices as in Theorem 4.2, we obtain the required result, since there are $\frac{|w|_a(|w|_a-1)+|w|_b(|w|_b-1)}{2}$ pairs of vertices at distance 2 in $G(w)$ while there are $|w|_a|w|_b - |w|_{ab}$ pairs of vertices at distance 3. It is to be noted that pairs of vertices at distance 1 contribute value 1 to the product defining $\pi(G(w))$. \square

Corollary 4.7. *The multiplicative Wiener index of a Parikh word representable graph $G(w)$ for a fair word $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is*

$$\pi(G(w)) = 2^{\frac{|w|^2-|w|}{2}} \left(\frac{3}{2}\right)^{|w|_{ab}}.$$

Proof. For a binary word w , we have $|w|_{ab} + |w|_{ba} = |w|_a|w|_b$. Since w is a fair word, $|w|_{ab} = |w|_{ba}$ so that $|w|_a|w|_b - 2|w|_{ab} = |w|_{ba} - |w|_{ab} = 0$. Also $|w| = |w|_a + |w|_b$. Hence from Theorem 4.6, $\pi(G(w)) = 2^{\frac{|w|^2-|w|}{2}} \left(\frac{3}{2}\right)^{|w|_{ab}}$. \square

Lemma 4.8. *Given a fixed value of e and of l , the maximum value of $\pi(G(w))$ over all Parikh word representable graphs of the form $G(w)$ for $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, with e edges, is attained on $G(ab^{l-1}a^{e-l}b)$.*

Proof. Since $|w|_b = l$ and the number of edges in $G(w)$ is $e = |w|_{ab}$, we have $|w|_a \leq e - l + 1$ as $G(w)$ is a connected graph with $|w|_a + |w|_b$ vertices so that $e \geq |w|_a + |w|_b - 1$. Note that in a connected graph G with n vertices and e edges, $e \geq n - 1$ [5]. Hence from Theorem 4.6, the multiplicative Wiener index of $G(w)$ is

$$\begin{aligned} \pi(G(w)) &= 2^{\frac{|w|_a(|w|_a-1)+|w|_b(|w|_b-1)}{2}} 3^{|w|_a|w|_b-|w|_{ab}} \\ &\leq 2^{\frac{(e-l+1)(e-l)+l(l-1)}{2}} 3^{(e-l+1)l-e} \end{aligned}$$

which is the multiplicative Wiener index of the Parikh word representable graph $G(ab^{l-1}a^{e-l}b)$. \square

Theorem 4.9. *An upper bound of the multiplicative Wiener index $\pi(G(w))$ of a Parikh word representable graph $G(w)$, $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, with e edges is given by*

$$\pi(G(w)) \leq \begin{cases} 2^{m^2-m}3^{m^2-2m+1} (m \geq 1), & \text{if } e = 2m - 1; \\ 2^{m^2}3^{m^2-m} (m \geq 1), & \text{if } e = 2m. \end{cases}$$

The bound is sharp and is attained on $G(ab^{m-1}a^{m-1}b)$ when $e = 2m - 1$ and on $G(ab^{m-1}a^m b)$ when $e = 2m$.

Proof. From Lemma 4.8, the multiplicative Wiener index of the Parikh word representable graph $G(w)$, $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, has a maximum for $G(ab^{l-1}a^{e-l}b)$ and is given by

$$\pi(G(w)) = 2^{\frac{(e-l+1)(e-l)+l(l-1)}{2}} 3^{(e-l+1)l-e}.$$

On taking logarithms we get,

$$\begin{aligned} \ln(\pi(G(w))) &= [(e - l + 1)(e - l) + l^2 - l] \frac{\ln 2}{2} + [(e - l + 1)l - e] \ln 3 \\ &= l^2(\ln 2 - \ln 3) - l((e + 1)(\ln 2 - \ln 3) + e \left(\frac{(e + 1)}{2} \ln 2 - \ln 3 \right)). \end{aligned}$$

We now use the fact that a quadratic expression $ax^2 + bx + c$, $a < 0$, has a maximum when $x = -\frac{b}{2a}$. Let $F(l) = l^2(\ln 2 - \ln 3) - l((e + 1)(\ln 2 - \ln 3) + e(\frac{e+1}{2} \ln 2 - \ln 3))$. When $e = 2m - 1, m \geq 1$, $F(l)$ has a maximum when $l = m$ and so $\pi(G(w))$ has the maximum $2^{m^2-m}3^{m^2-2m+1}$. When $e = 2m, m \geq 1$, $F(l)$ has a maximum when $l = [m + \frac{1}{2}] = m$ where $[x]$ is the integral part of x and $\pi(G(w))$ has the maximum $2^{m^2}3^{m^2-m}$. \square

Theorem 4.10. *The multiplicative Wiener index $\pi(G(w))$ of a Parikh word representable graph $G(w) = (V_1 \cup V_2, E)$ with $|V_1| = |w|_a = p, |V_2| = |w|_b = q$ for the word $w = a^{n_1}ba^{n_2}b \cdots a^{n_q}b$, $n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is bounded above by*

$$2^{\frac{p(p-1)+q(q-1)}{2}} 3^{pq-p-q+1}$$

and below by

$$2^{\frac{p(p-1)+q(q-1)}{2}}.$$

The bounds are attained on $G(ab^{q-1}a^{p-1}b)$ and $G(a^p b^q)$ respectively.

Proof. Since $G(w)$ is connected, $|w|_{ab} = |E| \geq p + q - 1$ [5]. Also $|w|_{ab} \leq pq$ [26]. Hence from Theorem 4.6, the multiplicative Wiener index of $G(w)$ is

$$\pi(G(w)) \geq 2^{\frac{p(p-1)+q(q-1)}{2}}$$

which is the multiplicative Wiener index of the Parikh word representable graph $G(a^p b^q)$ and

$$\pi(G(w)) \leq 2^{\frac{p(p-1)+q(q-1)}{2}} 3^{pq-p-q+1}$$

which is the multiplicative Wiener index of the Parikh word representable graph $G(ab^{q-1} a^{p-1}b)$. \square

5 Hyper-Wiener index of Parikh word representable graphs

We now derive formulas for computing hyper-Wiener index of Parikh word representable graphs of binary words.

Definition 5.1 ([20, 30]). The hyper-Wiener index of a connected graph G is given by

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) + d^2(u,v)$$

where $d(u,v)$ is the distance between the vertices u and v of G .

Theorem 5.2. *The hyper-Wiener index $WW(G(w))$ of a Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, is*

$$WW(G(w)) = 3 \left(\sum_{i=1}^l n_i \right)^2 + \sum_{i=1}^l (2l + 10i - 13)n_i + 3l(l - 1).$$

Proof. As in the proof of Theorem 3.2, there are four cases for the vertex pairs (u, v) . The contribution to the hyper-Wiener index of the Parikh word representable graph from each of these cases may be calculated as follows:

- (i) The contribution from pairs of vertices labeled a is

$$(n_1 + n_2 + \cdots + n_l)C_2 \times (2 + 4) = 3(n_1 + n_2 + \cdots + n_l)^2 - 3(n_1 + n_2 + \cdots + n_l).$$

- (ii) The contribution from pairs of vertices (u, v) where u is labeled a and v is labeled b is

$$2(n_1 + (n_1 + n_2) + \cdots + (n_1 + n_2 + \cdots + n_l)) = 2(ln_1 + (l - 1)n_2 + \cdots + n_l).$$

- (iii) The contribution from pairs of vertices (u, v) where u is labeled b and v is labeled a is

$$12(n_2 + 2n_3 + \cdots + (l - 1)n_l).$$

- (iv) The contribution from pairs of vertices labeled b is

$$lC_2 \times 6 = 3l(l - 1).$$

Hence the hyper-Wiener index of $G(w)$ is given by

$$WW(G(w)) = 3 \left(\sum_{i=1}^l n_i \right)^2 + \sum_{i=1}^l (2l + 10i - 13)n_i + 3l(l - 1). \quad \square$$

We now derive an alternate form of the expression for the hyper-Wiener index of the Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$.

Theorem 5.3. *The hyper-Wiener index of a Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, is*

$$\begin{aligned} WW(G(w)) &= 3|w|_a^2 + 3|w|_b^2 + 12|w|_a|w|_b - 3|w|_a - 3|w|_b - 10|w|_{ab} \\ &= 3|w|^2 - 3|w| + 6|w|_a|w|_b - 10|w|_{ab}. \end{aligned}$$

Proof. Since $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$, we have $\sum_{i=1}^l n_i = |w|_a$, $l = |w|_b$. Also, as in the proof of Theorem 3.4,

$$\sum_{i=1}^l in_i = |w|_a|w|_b + |w|_a - |w|_{ab}.$$

Hence from Theorem 5.2, the hyper-Wiener index

$$\begin{aligned} WW(G(w)) &= 3|w|_a^2 + (2|w|_b - 13)|w|_a + 3|w|_b(|w|_b - 1) + 10 \sum_{i=1}^l in_i \\ &= 3|w|_a^2 + 3|w|_b^2 + 12|w|_a|w|_b - 3|w|_a - 3|w|_b - 10|w|_{ab} \\ &= 3|w|^2 - 3|w| + 6|w|_a|w|_b - 10|w|_{ab} \end{aligned}$$

using $|w| = |w|_a + |w|_b$. □

Theorem 5.4. *The hyper-Wiener index of a Parikh word representable graph $G(w) = (V_1 \cup V_2, E)$ with $|V_1| = |w|_a = p$, $|V_2| = |w|_b = q$ for the word $w = a^{n_1}ba^{n_2}b \cdots a^{n_q}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, is bounded above and below by*

$$3(p^2 + q^2) + 12pq - 13p - 13q + 10$$

and

$$3(p^2 + q^2) + 2pq - 3p - 3q.$$

The bounds are attained on $G(ab^{q-1}a^{p-1}b)$ and $G(a^pb^q)$ respectively.

Proof. As done in the proof of Theorem 3.6, using the inequalities $|w|_{ab} \geq p + q - 1$ [5], $|w|_{ab} \leq pq$ [26], we have from Theorem 5.3, the hyper-Wiener index of $G(w)$ is

$$\begin{aligned} WW(G(w)) &= 3p^2 + 3q^2 + 12pq - 3p - 3q - 10|w|_{ab} \\ &\leq 3(p^2 + q^2) + 12pq - 13p - 13q + 10 \end{aligned}$$

which is the hyper-Wiener index of the Parikh word representable graph $G(ab^{q-1}a^{p-1}b)$ and

$$W(G(w)) \geq 3(p^2 + q^2) + 2pq - 3p - 3q$$

which is the Wiener index of the Parikh word representable graph $G(a^pb^q)$. □

The hyper-Wiener index of a Parikh word representable graph corresponding to a specific partition of a given integer can be evaluated proceeding as in the proof of Theorem 3.10 and is given in the following theorem.

Theorem 5.5. *Suppose $m_1 + m_2 + \dots + m_l$ is a partition of some positive integer, where $m_1 \geq m_2 \geq \dots \geq m_l \geq 1$. Then the hyper-Wiener index of the Parikh word representable graph G corresponding to this partition is given by*

$$WW(G) = 3(m_1^2 + (4l - 1)m_1 + l(l - 1)) - 10e$$

where e is the number of edges of G .

We shall now find an expression for an upper bound on the hyper-Wiener index of Parikh word representable graph with a fixed number of edges. We use the following lemma.

Lemma 5.6. *Given a fixed value of e and of l , the maximum value of $WW(G(w))$ over all Parikh word representable graphs of the form $G(w)$ for $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, with e edges, is attained on $G(ab^{l-1}a^{e-l}b)$.*

Proof. Proceeding as done in the proof of Lemma 3.8, the number of edges in $G(w)$ is $e = |w|_{ab}$, $|w|_b = l$ and $e \geq |w|_a + |w|_b - 1$ as $G(w)$ is a connected graph with $|w|_a + |w|_b$ vertices, we have $|w|_a \leq e - l + 1$. Hence from Theorem 5.3, the hyper-Wiener index of $G(w)$ is

$$\begin{aligned} WW(G(w)) &= 3|w|_a(|w|_a - 1) + 3l^2 + 12l|w|_a - 3l - 10e \\ &\leq 3(e - l + 1)(e - l) + 3l^2 + 12l(e - l + 1) - 3l - 10e \\ &= 3e^2 - 6l^2 + 6el + 6l - 7e \end{aligned}$$

which is the hyper-Wiener index of the Parikh word representable graph $G(ab^{l-1}a^{e-l}b)$. □

Theorem 5.7. *An upper bound of the Wiener index $W(G(w))$ of a Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, with e edges is given by*

$$WW(G) \leq \begin{cases} 18m^2 - 26m + 10 (m \geq 1), & \text{if } e = 2m - 1; \\ 18m^2 - 8m (m \geq 1), & \text{if } e = 2m. \end{cases}$$

The bound is sharp and is attained on $G(ab^{m-1}a^{m-1}b)$ when $e = 2m - 1$ and on $G(ab^{m-1}a^m b)$ when $e = 2m$.

Proof. From Lemma 5.6, the hyper-Wiener index of the Parikh word representable graph $G(w)$, $w = a^{n_1}ba^{n_2}b \dots a^{n_l}b$, $n_1 \geq 1$, has a maximum for $G(w)$ for $w = ab^{l-1}a^{e-l}b$ and is given by $WW(G(w)) = 3e^2 - 6l^2 + 6el + 6l - 7e$. We use the fact that a quadratic expression $ax^2 + bx + c$, $a < 0$, has a maximum when $x = -\frac{b}{2a}$. When $e = 2m - 1$, $m \geq 1$, we have $WW(G(w)) = -6l^2 + 12ml + (12m^2 - 26m + 10)$. If $e = 2m - 1$ has a fixed value, this quadratic expression in l has a maximum when $l = m$ and the maximum is $18m^2 - 26m + 10$. When $e = 2m$, $m \geq 1$, we have $WW(G(w)) = -6l^2 + l(6 + 12m) + (12m^2 - 14m)$. Again if $e = 2m$ has a fixed value, this quadratic expression has a maximum when $l = [m + \frac{1}{2}] = m$ where $[x]$ is the integral part of x and the maximum is $18m^2 - 8m$. □

6 Terminal and peripheral Wiener indices

By considering only pendant vertices in a graph, a special kind of Wiener index, called terminal Wiener index, has been introduced and studied [11]. Here we consider this notion in the context of Parikh word representable graphs.

Definition 6.1 ([11]). The terminal Wiener index $TW(G)$ of a connected graph G is the sum of distances between all pairs of pendant vertices of G .

Theorem 6.2. *The terminal Wiener index of a Parikh word representable graph $G = G(a^{n_1}ba^{n_2}b \dots a^{n_l}b)$, $n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is given by*

$$TW(G) = \begin{cases} n_l(n_l - 1), & \text{if } n_1 \neq 1; \\ n_l(n_l - 1) + k(k - 1) + 3kn_l, & \text{if } n_1 = 1, \text{ for } 2 \leq j \leq k \leq l, n_j = 0. \end{cases}$$

Proof. If $n_1 \neq 1$, the only possible pendant vertices are the a 's in the last block and the distance between any two of them is 2 so that

$$TW(G) = 2 \times n_l C_2 = n_l(n_l - 1).$$

Note that if $n_l = 0$, then $TW(G) = 0$.

If $n_1 = 1, n_2 = n_3 = \dots = n_k = 0$ and $n_{k+1} \neq 0, 2 \leq k < l, l > 1$, then the first k b 's are also a pendant vertices and the distance between any one of these b 's and any one of the a 's in the last block is 3 while that between any two b 's is 2 as well as the distance between any two a 's in the last block is 2. Hence

$$TW(G) = n_l(n_l - 1) + k(k - 1) + 3kn_l.$$

When $k = l$, then $n_1 = 1$ and $n_i = 0, 2 \leq i \leq l$ so that all the b 's are the only pendant vertices and hence

$$TW(G) = l(l - 1).$$

If $n_1 = 1, l = 1$, clearly $TW(G) = 1$ as the corresponding graph $G(ab)$ has only one edge with the end labels a and b . □

Another special kind of Wiener index, called peripheral Wiener index, has also been studied [16].

Definition 6.3 ([16]). The peripheral Wiener index of a connected graph G is given by $W_p(G) = \sum_{\{u,v\} \subseteq P(G)} d(u,v)$ where $P(G)$ is the set of all peripheral vertices which are the vertices of G with their eccentricities equal to diameter of G .

Theorem 6.4. *The peripheral Wiener index of the Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}ba^{n_3}b \dots a^{n_r}b^{l-r+1}$, $n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq r - 1$, and $n_r > 0$ with r at least 2 and at the most l , is*

$$PW(G(w)) = \left(\sum_{i=2}^r n_i \right)^2 + \sum_{i=2}^r (r + 2i - 4)n_i + (r - 1)(r - 2).$$

Furthermore $PW(G(w)) = W(G(w))$ if $w = a^n b^l$, where $W(G(w))$ is the Wiener index of $G(w)$.

Proof. From the definition of $G(w)$, the Parikh word representable graph corresponding to the word $w = a^{n_1}ba^{n_2}ba^{n_3}b \cdots a^{n_r}b^{l-r+1}$, it is clear that $G(w)$ is a bipartite graph of diameter 3 and radius 2. Also, the vertices corresponding to all a^i 's, $2 \leq i \leq r$ and to all b^i 's except the last $l - r + 1$ b^i 's are of eccentricity 3 and hence they are the peripheral vertices of $G(w)$. We consider pairs of peripheral vertices (u, v) , where the label of u appears before the label of v in w . As in Theorem 3.2, the vertex pairs of (u, v) can be divided into four cases as given below:

1. u and v are both labeled a ;
2. u is labeled a and v is labeled b ;
3. u is labeled b and v is labeled a ;
4. u and v are both labeled b .

The contribution to the peripheral Wiener index of the Parikh word representable graph from each of these cases may be calculated as follows:

1. The contribution from the pairs of peripheral vertices labeled a is

$$(n_2+n_3+n_4+\cdots+n_r)C_2 \times 2 = (n_2+n_3+n_4+\cdots+n_r)^2 - (n_2+n_3+n_4+\cdots+n_r).$$

2. The contribution from the pairs of peripheral vertices (u, v) where u is labeled a and v is labeled b is

$$\begin{aligned} n_2 + (n_2 + n_3) + (n_2 + n_3 + n_4) + \cdots + (n_2 + n_3 + \cdots + n_{r-1}) \\ = (r - 2)n_2 + (r - 3)n_3 + \cdots + n_{r-1}. \end{aligned}$$

3. The contribution from the pairs of peripheral vertices (u, v) where u is labeled b and v is labeled a is

$$\begin{aligned} 3[(n_2 + n_3 + \cdots + n_r) + (n_3 + n_4 + \cdots + n_r) + \cdots + n_r] \\ = 3[(r - 1)n_r + (r - 2)n_{r-1} + \cdots + n_2]. \end{aligned}$$

4. The contribution from the pairs of peripheral vertices labeled b is

$$(r - 1)C_2 \times 2 = (r - 1)(r - 2).$$

Hence the peripheral Wiener index of $G(w)$ is given by


$$PW(G(w)) = \left(\sum_{i=2}^r n_i \right)^2 + \sum_{i=2}^r (r + 2i - 4)n_i + (r - 1)(r - 2).$$


Furthermore, if $w = a^n b^l$ then all the vertices of $G(w)$ labeled a as well as b are peripheral vertices of $G(w)$. Thus $PW(G(w)) = W(G(w))$ where $W(G(w))$ is the Wiener index of $G(w)$. □


7 Conclusion


We have derived formulas for evaluating the Wiener index and certain other variants of Wiener topological indices for Parikh word representable graphs [3] of binary core words. There are problems that remain to be investigated. For example, the lower bound of Wiener index of a Parikh word representable graph $G(w)$ of a binary core word w when the number of edges of $G(w)$ is a given fixed value, needs to be examined. Bipartite graphs have been utilized in studies of structural features in the areas of molecular biology and chemistry (see, for example, [17, 35]). Parikh word representable graphs (*PWRG*) corresponding to binary core words are bipartite graphs. It will be of interest to examine the role of *PWRG* in such studies of structural features and relationships. Also, it will also be of interest to study other kinds of topological indices for this class of graphs.

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A double Sylvester determinant*

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Abstract

Given two $(n + 1) \times (n + 1)$ -matrices A and B over a commutative ring, and some $k \in \{0, 1, \dots, n\}$, we consider the $\binom{n}{k} \times \binom{n}{k}$ -matrix W whose entries are $(k + 1) \times (k + 1)$ -minors of A multiplied by corresponding $(k + 1) \times (k + 1)$ -minors of B . Here we require the minors to use the last row and the last column (which is why we obtain an $\binom{n}{k} \times \binom{n}{k}$ -matrix, not a $\binom{n+1}{k+1} \times \binom{n+1}{k+1}$ -matrix). We prove that the determinant $\det W$ is a multiple of $\det A$ if the $(n + 1, n + 1)$ -th entry of B is 0. Furthermore, if the $(n + 1, n + 1)$ -th entries of both A and B are 0, then $\det W$ is a multiple of $(\det A) (\det B)$. This extends a previous result of Olver and the author.

Keywords: Determinant, compound matrix, Sylvester’s determinant, polynomials.

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1 Introduction

Let n and k be nonnegative integers, and let $A = (a_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1}$ be an $(n + 1) \times (n + 1)$ -matrix over some commutative ring. Let P_k be the set of all k -element subsets of $\{1, 2, \dots, n\}$. For any such subset $K \in P_k$, let $K+$ denote the subset $K \cup \{n + 1\}$ of $\{1, 2, \dots, n + 1\}$. If U and V are two subsets of $\{1, 2, \dots, n + 1\}$, then $\text{sub}_U^V A$ shall denote the $|U| \times |V|$ -submatrix of A containing only the entries $a_{u,v}$ with $u \in U$ and $v \in V$. Let W_A be the $P_k \times P_k$ -matrix¹ whose (I, J) -th entry (for all $I \in P_k$ and $J \in P_k$) is

$$\det \left(\text{sub}_{I+}^{J+} A \right).$$

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¹This means a matrix whose rows and columns are indexed by the k -element subsets of $\{1, 2, \dots, n\}$. If you pick a total order on the set P_k , then you can view such a matrix as an $\binom{n}{k} \times \binom{n}{k}$ -matrix.

(Thus, the entries of W_A are all $(k + 1) \times (k + 1)$ -minors of A that use the last row and the last column.) A particular case of a celebrated result going back to Sylvester [15] (see [12, §2.7] or [13, Teorema 2.9.1] or [10] for modern proofs) then says that

$$\det(W_A) = a_{n+1,n+1}^p \cdot (\det A)^q, \quad \text{where } p = \binom{n-1}{k} \text{ and } q = \binom{n-1}{k-1}.$$

Now, consider a second $(n + 1) \times (n + 1)$ -matrix $B = (b_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1}$ over the same ring. Let $W_{A,B}$ (later to be just called W) be the $P_k \times P_k$ -matrix whose (I, J) -th entry (for all $I \in P_k$ and $J \in P_k$) is

$$\det(\text{sub}_{I+}^{J+} A) \det(\text{sub}_{I+}^{J+} B).$$

What can be said about $\det(W_{A,B})$? In general, very little². However, under some assumptions, it splits off factors. Namely, we shall show (Theorem 2.1) that $\det(W_{A,B})$ is a multiple of $\det A$ if $b_{n+1,n+1} = 0$. We shall then conclude (Theorem 2.2) that if both $a_{n+1,n+1}$ and $b_{n+1,n+1}$ are 0, then $\det(W_{A,B})$ is a multiple of $(\det A)(\det B)$. In either case, the quotient (usually a much more complicated polynomial³) remains mysterious; our proofs are indirect and reveal little about it. Our second result generalizes a curious property of $\binom{n}{2} \times \binom{n}{2}$ -determinants [6, Theorem 10] that arose from the study of the n -body problem (see Example 2.4 for details).

2 The theorems

Let us first introduce the standing notations.

Let $\mathbb{N} = \{0, 1, 2, \dots\}$. Let \mathbb{K} be a commutative ring. If a and b are two elements of \mathbb{K} , then we write $a \mid b$ when b is a multiple of a (that is, $b \in \mathbb{K}a$).

If $m \in \mathbb{N}$, then $[m]$ shall mean the set $\{1, 2, \dots, m\}$.

Fix an $n \in \mathbb{N}$. If K is any subset of $[n]$, then $K+$ shall mean the subset $K \cup \{n + 1\}$ of $[n + 1]$.

Fix $k \in \{0, 1, \dots, n\}$. Let P_k be the set of all k -element subsets of $[n]$. This is a finite set; thus, any $P_k \times P_k$ -matrix (i.e., any matrix whose rows and columns are indexed by k -element subsets of $[n]$) has a well-defined determinant⁴. Such matrices appear frequently in classical determinant theory (see, e.g., the “ k -th compound determinants” in [11] and in [12, §2.6], as well as the related “Generalized Sylvester’s identity” in [12, §2.7] and [13, Teorema 2.9.1] and [10]).

If $A \in \mathbb{K}^{u \times v}$ is a $u \times v$ -matrix, and if $I \subseteq [u]$ and $J \subseteq [v]$, then $\text{sub}_I^J A$ shall mean the submatrix of A obtained by removing all rows whose indices are not in I and removing all columns whose indices are not in J . (Rigorously speaking, if $A = (a_{i,j})_{1 \leq i \leq u, 1 \leq j \leq v}$ and $I = \{i_1 < i_2 < \dots < i_p\}$ and $J = \{j_1 < j_2 < \dots < j_q\}$, then $\text{sub}_I^J A$ is defined to be the matrix $(a_{i_x, j_y})_{1 \leq x \leq p, 1 \leq y \leq q}$.) When $|I| = |J|$, then the submatrix $\text{sub}_I^J A$ is square; its determinant $\det(\text{sub}_I^J A)$ is called a *minor* of A .

²For example, if $n = 3$ and $k = 2$, then $\det(W_{A,B})$ is an irreducible polynomial in the (altogether $2(n + 1)^2 = 32$) variables $a_{i,j}$ and $b_{i,j}$ with 110268 monomials.

³Again, irreducible in the case when $n = 3$ and $k = 2$.

⁴Here, we are using the concepts of $P \times P$ -matrices (where P is a finite set) and their determinants. Both of these concepts are folklore; a brief introduction can be found in [5, §1].

Our main two results are the following:

Theorem 2.1. *Let*

$$A = (a_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1} \in \mathbb{K}^{(n+1) \times (n+1)} \quad \text{and}$$

$$B = (b_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1} \in \mathbb{K}^{(n+1) \times (n+1)}$$

be such that $b_{n+1,n+1} = 0$. Let W be the $P_k \times P_k$ -matrix whose (I, J) -th entry (for all $I \in P_k$ and $J \in P_k$) is

$$\det(\text{sub}_{I^+}^{J^+} A) \det(\text{sub}_{I^+}^{J^+} B).$$

Then $\det A \mid \det W$.

Theorem 2.2. *Let*

$$A = (a_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1} \in \mathbb{K}^{(n+1) \times (n+1)} \quad \text{and}$$

$$B = (b_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1} \in \mathbb{K}^{(n+1) \times (n+1)}$$

be such that $a_{n+1,n+1} = 0$ and $b_{n+1,n+1} = 0$. Define the $P_k \times P_k$ -matrix W as in Theorem 2.1. Then $(\det A) (\det B) \mid \det W$.

Example 2.3. For this example, set $k = 1$. Then $P_k = P_1 = \{\{1\}, \{2\}, \dots, \{n\}\}$. Thus, the map

$$[n] \rightarrow P_k, \quad i \mapsto \{i\}$$

is a bijection. Use this bijection to identify the elements $1, 2, \dots, n$ of $[n]$ with the elements $\{1\}, \{2\}, \dots, \{n\}$ of P_k . Thus, the $P_k \times P_k$ -matrix W in Theorem 2.1 becomes the $n \times n$ -matrix

$$\left(\underbrace{\det(\text{sub}_{\{i\}^+}^{\{j\}^+} A)}_{\substack{=a_{i,j}a_{n+1,n+1} \\ -a_{i,n+1}a_{n+1,j}}} \underbrace{\det(\text{sub}_{\{i\}^+}^{\{j\}^+} B)}_{\substack{=b_{i,j}b_{n+1,n+1} \\ -b_{i,n+1}b_{n+1,j}}} \right)_{1 \leq i \leq n, 1 \leq j \leq n}$$

$$= \left((a_{i,j}a_{n+1,n+1} - a_{i,n+1}a_{n+1,j}) \underbrace{(b_{i,j}b_{n+1,n+1} - b_{i,n+1}b_{n+1,j})}_{=0} \right)_{1 \leq i \leq n, 1 \leq j \leq n}$$

$$= ((a_{i,j}a_{n+1,n+1} - a_{i,n+1}a_{n+1,j})(-b_{i,n+1}b_{n+1,j}))_{1 \leq i \leq n, 1 \leq j \leq n}.$$

This is the matrix obtained from $(a_{i,j}a_{n+1,n+1} - a_{i,n+1}a_{n+1,j})_{1 \leq i \leq n, 1 \leq j \leq n}$ by multiplying the i -th row with $-b_{i,n+1}$ for all $i \in [n]$ and multiplying the j -th column with $b_{n+1,j}$ for all $j \in [n]$. Thus, the claim of Theorem 2.1 follows from the classical fact that

$$\det \left((a_{i,j}a_{n+1,n+1} - a_{i,n+1}a_{n+1,j})_{1 \leq i \leq n, 1 \leq j \leq n} \right) = a_{n+1,n+1}^{n-1} \cdot \det A.$$

This fact is known as Chio pivotal condensation (see, e.g., [7, Theorem 0.1]), and is a particular case of Sylvester’s identity ([12, §2.7]).

Example 2.4. For this example, set $k = 2$, and consider the situation of Theorem 2.1 again. Then $P_k = P_2 = \{\{i, j\} \mid 1 \leq i < j \leq n\}$. If $\{i, j\} \in P_2$ and $\{k, l\} \in P_2$ satisfy $i < j$ and $k < l$, then the $(\{i, j\}, \{k, l\})$ -th entry of W is

$$\det(\text{sub}_{\{i,j\}^+}^{\{k,l\}^+} A) \det(\text{sub}_{\{i,j\}^+}^{\{k,l\}^+} B) = \det \begin{pmatrix} a_{i,k} & a_{i,l} & a_{i,n+1} \\ a_{j,k} & a_{j,l} & a_{j,n+1} \\ a_{n+1,k} & a_{n+1,l} & a_{n+1,n+1} \end{pmatrix} \det \begin{pmatrix} b_{i,k} & b_{i,l} & b_{i,n+1} \\ b_{j,k} & b_{j,l} & b_{j,n+1} \\ b_{n+1,k} & b_{n+1,l} & 0 \end{pmatrix}.$$

Note that $b_{n+1,n+1} = 0$. If we furthermore assume that

$$\begin{aligned} a_{n+1,n+1} &= 0, & \text{and} \\ a_{n+1,i} &= a_{i,n+1} = 1 \quad \text{for all } i \in [n], & \text{and} \\ b_{n+1,i} &= b_{i,n+1} = 1 \quad \text{for all } i \in [n], \end{aligned}$$

then this entry rewrites as

$$\det \begin{pmatrix} a_{i,k} & a_{i,l} & 1 \\ a_{j,k} & a_{j,l} & 1 \\ 1 & 1 & 0 \end{pmatrix} \det \begin{pmatrix} b_{i,k} & b_{i,l} & 1 \\ b_{j,k} & b_{j,l} & 1 \\ 1 & 1 & 0 \end{pmatrix} = (a_{j,k} + a_{i,l} - a_{i,k} - a_{j,l})(b_{j,k} + b_{i,l} - b_{i,k} - b_{j,l}).$$

Hence, [6, Theorem 10] can be obtained from Theorem 2.2 by setting $k = 2$ and $A = C_S$ and $B = C_T$ (and observing that the matrix W then equals to $W_{S,T}$).

3 The proofs

Our proofs of Theorem 2.1 and Theorem 2.2 will rely on some basic commutative algebra: the notion of a unique factorization domain (“UFD”); the concepts of coprime, prime and irreducible elements; the localization of a commutative ring at a multiplicative subset. This all appears in most textbooks on abstract algebra; for example, [8, Sections VIII.4 and VIII.10] is a good reference⁵.

The *content* of a polynomial p over a UFD is defined to be the greatest common divisor of the coefficients of p . For example, the polynomial $4x^2 + 6y^2 \in \mathbb{Z}[x, y]$ has content $\gcd(4, 6) = 2$. (Of course, in a general UFD, the greatest common divisor is defined only up to multiplication by a unit.) The following known facts are crucial to us:

Proposition 3.1. *A polynomial ring over \mathbb{Z} in finitely many indeterminates is always a UFD.* □

Proposition 3.1 appears, e.g., in [8, Remark after Corollary 8.21]. For a constructive proof of Proposition 3.1, we refer to [9, Chapter IV, Theorems 4.8 and 4.9] or to [2, Essay 1.4, Corollary of Theorem 1 and Corollary 1 of Theorem 2].

Proposition 3.2. *Let p be an irreducible element of a UFD \mathbb{K} . Then the quotient ring $\mathbb{K}/(p)$ is an integral domain.*

⁵We call “multiplicative subset” what Knapp (in [8, Section VIII.10]) calls a “multiplicative system”.

Proof of Proposition 3.2. First of all, we recall that any irreducible element of a UFD is prime (indeed, this follows from [8, Proposition 8.13]). Thus, the element p of \mathbb{K} is prime. Hence, [8, Proposition 8.14] shows that the ideal (p) of \mathbb{K} is prime. Therefore, the quotient ring $\mathbb{K}/(p)$ is an integral domain. This proves Proposition 3.2. \square

We shall furthermore use the following properties of contents (whose proofs are easy):

Proposition 3.3. *Let \mathbb{U} be a UFD. Let $p \in \mathbb{U}[x_1, x_2, \dots, x_m]$ be a polynomial over \mathbb{U} . Assume that the content of p is 1. Also assume that p is irreducible when considered as a polynomial in $\mathbb{F}[x_1, x_2, \dots, x_m]$, where \mathbb{F} is the field of fractions of \mathbb{U} . Then p is also irreducible when considered as a polynomial in $\mathbb{U}[x_1, x_2, \dots, x_m]$.*

Proposition 3.4. *Let \mathbb{U} be a UFD. Let $p, q \in \mathbb{U}[x_1, x_2, \dots, x_m]$ be two polynomials over \mathbb{U} . Assume that both p and q have content 1, and assume furthermore that p and q don't have any indeterminates in common (i.e., there is no $i \in [m]$ such that $\deg_{x_i} p > 0$ and $\deg_{x_i} q > 0$). Then p and q are coprime.*

The next simple fact states that for any positive integer n , the determinant of the “generic $n \times n$ -matrix” (i.e., of the $n \times n$ -matrix whose n^2 entries are distinct indeterminates in a polynomial ring over \mathbb{Z}) is irreducible as a polynomial over \mathbb{Z} :

Corollary 3.5. *Let n be a positive integer. Let \mathbb{G} be the multivariate polynomial ring $\mathbb{Z}[a_{i,j} \mid (i, j) \in [n]^2]$. Let $\bar{A} \in \mathbb{G}^{n \times n}$ be the $n \times n$ -matrix $(a_{i,j})_{1 \leq i \leq n, 1 \leq j \leq n}$. Then the element $\det \bar{A}$ of \mathbb{G} is irreducible.*

Proof of Corollary 3.5. A well-known fact (e.g., [1, Lemma 5.12]) shows that $\det \bar{A}$ is irreducible as an element of $\mathbb{Q}[a_{i,j} \mid (i, j) \in [n]^2]$. This yields (using Proposition 3.3) that $\det \bar{A}$ is irreducible as an element of $\mathbb{Z}[a_{i,j} \mid (i, j) \in [n]^2]$ as well, since the polynomial $\det \bar{A}$ has content 1. This proves Corollary 3.5. \square

An element a of a commutative ring \mathbb{A} is said to be *regular* if every $b \in \mathbb{A}$ satisfying $ab = 0$ must satisfy $b = 0$. (Regular elements are also known as *non-zero-divisors*.) In a polynomial ring, each indeterminate is regular; hence, each monomial (without coefficient) is regular (since any product of two regular elements is regular).

We recall a few standard concepts from commutative algebra. Let \mathbb{K} be a commutative ring. A *multiplicative subset* of \mathbb{K} means a subset S of \mathbb{K} that contains the unity $1_{\mathbb{K}}$ of \mathbb{K} and has the property that every $a, b \in S$ satisfy $ab \in S$.

If S is a multiplicative subset of \mathbb{K} , then the *localization* of \mathbb{K} at S is defined as follows: Let \sim be the binary relation on the set $\mathbb{K} \times S$ defined by

$$((r, s) \sim (r', s')) \iff (t(rs' - sr') = 0 \text{ for some } t \in S).$$

Then it is easy to see that \sim is an equivalence relation. The set \mathbb{L} of its equivalence classes $[(r, s)]$ can be equipped with a ring structure via the rules $[(r, s)] + [(r', s')] = [(rs' + sr', ss')]$ and $[(r, s)] \cdot [(r', s')] = [(rr', ss')]$ (with zero element $[(0, 1)]$ and unity $[(1, 1)]$). The resulting ring \mathbb{L} is commutative, and is known as the localization of \mathbb{K} at S . (This generalizes the construction of \mathbb{Q} from \mathbb{Z} known from high school.)

The element $[(r, s)]$ of \mathbb{L} is denoted by $\frac{r}{s}$. There is a canonical ring homomorphism from \mathbb{K} to \mathbb{L} that sends each $r \in \mathbb{K}$ to $[(r, 1)] = \frac{r}{1} \in \mathbb{L}$.

When all elements of the multiplicative subset S are regular, the statement “ $t(rs' - sr') = 0$ for some $t \in S$ ” in the definition of the relation \sim can be rewritten in the equivalent (but much simpler) form “ $rs' = sr'$ ” (which is even more reminiscent of the construction of \mathbb{Q}).

The following fact is easy to see:

Proposition 3.6. *Let \mathbb{K} be a commutative ring. Let S be a multiplicative subset of \mathbb{K} such that all elements of S are regular. Let \mathbb{L} be the localization of the ring \mathbb{K} at S . Then:*

- (a) *The canonical ring homomorphism from \mathbb{K} to \mathbb{L} is injective. We shall thus consider it as an embedding.*
- (b) *If \mathbb{K} is an integral domain, then \mathbb{L} is an integral domain.*
- (c) *Let a and b be two elements of \mathbb{K} . Then we have the following logical equivalence:*

$$(a \mid b \text{ in } \mathbb{L}) \iff (a \mid sb \text{ in } \mathbb{K} \text{ for some } s \in S).$$

Matrices over arbitrary commutative rings can behave a lot less predictably than matrices over fields. However, matrices over integral domains still show a lot of the latter good behavior, such as the following:

Proposition 3.7. *Let P be a finite set. Let \mathbb{M} be an integral domain. Let $W \in \mathbb{M}^{P \times P}$ be a $P \times P$ -matrix over \mathbb{M} . Let $\mathbf{u} \in \mathbb{M}^P$ be a vector such that $\mathbf{u} \neq 0$ and $W\mathbf{u} = 0$. Here, \mathbf{u} is considered as a “column vector”, so that $W\mathbf{u}$ is defined by*

$$W\mathbf{u} = \left(\sum_{q \in P} w_{p,q} u_q \right)_{p \in P}, \quad \text{where } W = (w_{p,q})_{(p,q) \in P \times P} \quad \text{and} \quad \mathbf{u} = (u_p)_{p \in P}.$$

Then $\det W = 0$.

Proof of Proposition 3.7. Let $m = |P|$. Then we can view the $P \times P$ -matrix W as an $m \times m$ -matrix (by “numerical reindexing”, as explained in [5, §1]), and we can view the vector \mathbf{u} as a column vector of size m . Let us do this from here on.

Let \mathbb{F} be the quotient field of the integral domain \mathbb{M} . Thus, there is a canonical embedding of \mathbb{M} into \mathbb{F} . Hence, we can view the matrix $W \in \mathbb{M}^{m \times m}$ as a matrix over \mathbb{F} , and we can view the vector $\mathbf{u} \in \mathbb{M}^m$ as a vector over \mathbb{F} . Let us do so from here on. We are now in the realm of classical linear algebra over fields: The vector $\mathbf{u} \in \mathbb{F}^m$ is nonzero (since $\mathbf{u} \neq 0$) and belongs to the kernel of the $m \times m$ -matrix $W \in \mathbb{F}^{m \times m}$ (since $W\mathbf{u} = 0$). Hence, the kernel of the matrix W is nontrivial. In other words, this matrix W is singular. Thus, $\det W = 0$ by a classical fact of linear algebra. This proves Proposition 3.7. \square

Let us next recall an identity for determinants (a version of the Cauchy–Binet formula):

Lemma 3.8. *Let $n \in \mathbb{N}$, $m \in \mathbb{N}$ and $p \in \mathbb{N}$. Let $A \in \mathbb{K}^{n \times p}$ be an $n \times p$ -matrix. Let $B \in \mathbb{K}^{p \times m}$ be a $p \times m$ -matrix. Let $k \in \mathbb{N}$. Let P be a subset of $[n]$ such that $|P| = k$. Let Q be a subset of $[m]$ such that $|Q| = k$. Then*

$$\det(\text{sub}_P^Q(AB)) = \sum_{\substack{R \subseteq [p]; \\ |R|=k}} \det(\text{sub}_P^R A) \cdot \det(\text{sub}_R^Q B). \quad \square$$

Lemma 3.8 is [4, Corollary 7.251] (except that we are using the notation $\text{sub}_I^J C$ for what is called $\text{sub}_{w(I)}^{w(J)} C$ in [4]). It also appears in [3, Chapter I, (19)] (where it is stated using p -tuples instead of subsets).

The next lemma is just a particular case of Theorem 2.1, but it is a helpful stepping stone on the way to proving the latter theorem:

Lemma 3.9. *Let*

$$A = (a_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1} \in \mathbb{K}^{(n+1) \times (n+1)} \quad \text{and}$$

$$B = (b_{i,j})_{1 \leq i \leq n+1, 1 \leq j \leq n+1} \in \mathbb{K}^{(n+1) \times (n+1)}$$

be such that $b_{n+1,n+1} = 0$. Assume further that

$$a_{n+1,j} = 0 \quad \text{for all } j \in [n]. \tag{3.1}$$

Define the $P_k \times P_k$ -matrix W as in Theorem 2.1. Then $\det A \mid \det W$.

The following proof is inspired by [6, proof of Theorem 10].

Proof of Lemma 3.9. We WLOG assume that \mathbb{K} is the polynomial ring over \mathbb{Z} in $n^2 + (n + 1) + ((n + 1)^2 - 1)$ indeterminates

$$a_{i,j} \quad \text{for all } i \in [n] \text{ and } j \in [n];$$

$$a_{i,n+1} \quad \text{for all } i \in [n + 1];$$

$$b_{i,j} \quad \text{for all } i \in [n + 1] \text{ and } j \in [n + 1] \text{ except for } b_{n+1,n+1}.$$

And, of course, we assume that the entries of A and B that are not zero by assumption are these indeterminates.⁶

The ring \mathbb{K} is a UFD (by Proposition 3.1).

We WLOG assume that $n > 0$ (otherwise, the result follows from $\det W = \det(0) = 0$).

The set P_k is nonempty (since $k \in \{0, 1, \dots, n\}$); thus, $|P_k| \geq 1$.

Let \bar{A} be the $n \times n$ -matrix $(a_{i,j})_{1 \leq i \leq n, 1 \leq j \leq n} \in \mathbb{K}^{n \times n}$. Then, because of (3.1), we have

$$\det A = a_{n+1,n+1} \cdot \det \bar{A} \tag{3.2}$$

(by [4, Theorem 6.43], applied to $n + 1$ instead of n).

The matrix \bar{A} is a completely generic $n \times n$ -matrix (i.e., its entries are distinct indeterminates); thus, its determinant $\det \bar{A}$ is an irreducible polynomial in the polynomial ring $\mathbb{Z}[a_{i,j} \mid (i, j) \in [n]^2]$ (by Corollary 3.5). Hence, $\det \bar{A}$ also is an irreducible polynomial in the ring \mathbb{K} (since \mathbb{K} differs from $\mathbb{Z}[a_{i,j} \mid (i, j) \in [n]^2]$ only in having more variables, which clearly cannot contribute any factors to $\det \bar{A}$). Thus, Proposition 3.2 (applied to $p = \det \bar{A}$) shows that the quotient ring $\mathbb{K}/(\det \bar{A})$ is an integral domain.

Let \mathbb{M} be the quotient ring $\mathbb{K}/(\det \bar{A})$. Then \mathbb{M} is an integral domain (since $\mathbb{K}/(\det \bar{A})$ is an integral domain). All monomials in the variables $b_{i,j}$ (with $(i, j) \neq (n + 1, n + 1)$) are nonzero in \mathbb{M} . Likewise, $a_{n+1,n+1} \neq 0$ in \mathbb{M} .

⁶These assumptions are legitimate, because if we can prove Lemma 3.9 under these assumptions, then the universal property of polynomial rings shows that Lemma 3.9 holds in the general case.

Let w be the element $\prod_{j \in [n]} b_{n+1,j} \in \mathbb{M}$. (Strictly speaking, we mean the canonical projection of $\prod_{j \in [n]} b_{n+1,j} \in \mathbb{K}$ onto the quotient ring \mathbb{M} .) Then, w is a nonzero element of the integral domain \mathbb{M} (since $b_{n+1,j} \neq 0$ in \mathbb{M} for all $j \in [n]$).

For each $i \in [n]$, we define $z_i \in \mathbb{M}$ by $z_i = \prod_{j \in [n]; j \neq i} b_{n+1,j}$ (projected onto \mathbb{M}). This is a nonzero element of \mathbb{M} . In \mathbb{M} , we have

$$b_{n+1,i} z_i = b_{n+1} \prod_{\substack{j \in [n]; \\ j \neq i}} b_{n+1,j} = \prod_{j \in [n]} b_{n+1,j} = w \tag{3.3}$$

for all $i \in [n]$.

We need another piece of notation: If M is a $p \times q$ -matrix, and if $u \in [p]$ and $v \in [q]$, then $M_{\sim u, \sim v}$ denotes the $(p - 1) \times (q - 1)$ -matrix obtained from M by removing the u -th row and the v -th column.

The matrix $A_{\sim 1, \sim (n+1)}$ has determinant 0 (because (3.1) shows that its last row consists of zeroes). In other words, $\det(A_{\sim 1, \sim (n+1)}) = 0$.

Also, due to (3.1), we see that each $i \in [n]$ satisfies

$$\det(A_{\sim 1, \sim i}) = a_{n+1, n+1} \cdot \det(\overline{A}_{\sim 1, \sim i}) \tag{3.4}$$

(by [4, Theorem 6.43], applied to $A_{\sim 1, \sim i}$ instead of A), because the last row of the matrix $A_{\sim 1, \sim i}$ is $(0, 0, \dots, 0, a_{n+1, n+1})$.

For each $i \in [n + 1]$, we define an element $u_i \in \mathbb{M}$ by

$$u_i = \begin{cases} z_i (-1)^i \det(A_{\sim 1, \sim i}), & \text{if } i \in [n]; \\ 1, & \text{if } i = n + 1. \end{cases}$$

Claim 1. All these $n + 1$ elements u_1, u_2, \dots, u_{n+1} of \mathbb{M} are nonzero.

Proof of Claim 1. Let $i \in [n]$. Then, $\det(\overline{A}_{\sim 1, \sim i}) \neq 0$ in \mathbb{M} because $\det(\overline{A}_{\sim 1, \sim i})$ is a polynomial of smaller degree than $\det \overline{A}$, and thus is not a multiple of $\det \overline{A}$. Now,

$$\begin{aligned} u_i &= z_i (-1)^i \overbrace{\det(A_{\sim 1, \sim i})}^{= a_{n+1, n+1} \cdot \det(\overline{A}_{\sim 1, \sim i}) \quad \text{(by (3.4))}} \\ &= \underbrace{z_i}_{\neq 0 \text{ in } \mathbb{M}} \underbrace{(-1)^i}_{\neq 0 \text{ in } \mathbb{M}} \underbrace{a_{n+1, n+1}}_{\neq 0 \text{ in } \mathbb{M}} \cdot \underbrace{\det(\overline{A}_{\sim 1, \sim i})}_{\neq 0 \text{ in } \mathbb{M}} \\ &\neq 0 \text{ in } \mathbb{M} \quad (\text{since } \mathbb{M} \text{ is an integral domain}). \end{aligned}$$

Thus, u_1, u_2, \dots, u_n are nonzero. Moreover, u_{n+1} is nonzero (since $u_{n+1} = 1$). Thus, we are done. □

Let $\mathbf{u} = (u_J)_{J \in P_k} \in \mathbb{M}^{P_k}$ be the vector defined by

$$u_J = \prod_{j \in J} u_j.$$

Then the entries of the vector \mathbf{u} are nonzero (because they are products of the nonzero elements u_1, u_2, \dots, u_{n+1} of the integral domain \mathbb{M}). Since the vector \mathbf{u} has at least one entry (because $|P_k| \geq 1$), we thus conclude that $\mathbf{u} \neq 0$.

Let Δ be the diagonal matrix $\Delta = \text{diag}(u_1, u_2, \dots, u_{n+1}) \in \mathbb{M}^{(n+1) \times (n+1)}$.

Let $\mathbf{x} \in \mathbb{M}^{n+1}$ be the column vector defined by

$$\mathbf{x} = \left((-1)^1 \det(A_{\sim 1, \sim 1}), (-1)^2 \det(A_{\sim 1, \sim 2}), \dots, (-1)^{n+1} \det(A_{\sim 1, \sim (n+1)}) \right)^T.$$

Let $(e_1, e_2, \dots, e_{n+1})$ be the standard basis of the free \mathbb{M} -module \mathbb{M}^{n+1} . Thus, for any $(n+1) \times (n+1)$ -matrix $C \in \mathbb{M}^{(n+1) \times (n+1)}$ and any $j \in \{1, 2, \dots, n+1\}$, we have

$$(\text{the } j\text{-th column of the matrix } C) = C e_j. \tag{3.5}$$

Now, using Laplace expansion, it is easy to see that

$$A \mathbf{x} = -\det A \cdot e_1. \tag{3.6}$$

To prove Equation (3.6), consider the adjugate $\text{adj } A$ of the matrix A . A standard fact ([4, Theorem 6.100]) says that $A \cdot \text{adj } A = \det A \cdot I_{n+1}$. But the definition of $\text{adj } A$ reveals that the first column of the matrix $\text{adj } A$ is $-\mathbf{x}$. Hence, the first column of the matrix $A \cdot \text{adj } A$ is $A \cdot (-\mathbf{x}) = -A \mathbf{x}$. On the other hand, the first column of the matrix $A \cdot \text{adj } A$ is $\det A \cdot e_1$ (since $A \cdot \text{adj } A = \det A \cdot I_{n+1}$). Comparing the preceding two sentences, we conclude that $-A \mathbf{x} = \det A \cdot e_1$, so that $A \mathbf{x} = -\det A \cdot e_1$. This proves Equation (3.6).

Also, Equation (3.5) (applied to $C = B^T$ and $j = n+1$) yields

$$\begin{aligned} B^T e_{n+1} &= (\text{the } (n+1)\text{-st column of the matrix } B^T) \\ &= (b_{n+1,1}, b_{n+1,2}, \dots, b_{n+1,n+1})^T. \end{aligned}$$

Hence,

$$\begin{aligned} \Delta B^T e_{n+1} &= \Delta (b_{n+1,1}, b_{n+1,2}, \dots, b_{n+1,n+1})^T \\ &= (u_1 b_{n+1,1}, u_2 b_{n+1,2}, \dots, u_{n+1} b_{n+1,n+1})^T \end{aligned} \tag{3.7}$$

(since $\Delta = \text{diag}(u_1, u_2, \dots, u_{n+1})$).

Claim 2. We have

$$u_i b_{n+1,i} = w \cdot (-1)^i \det(A_{\sim 1, \sim i}) \quad \text{for each } i \in [n+1]. \tag{3.8}$$

Proof of Claim 2. Let $i \in [n+1]$. If $i = n+1$, then both sides of (3.8) are zero (because $b_{n+1,n+1} = 0$ and $\det(A_{\sim 1, \sim (n+1)}) = 0$). If $i \neq n+1$, then $i \in [n]$ and thus the definition of u_i yields $u_i = z_i (-1)^i \det(A_{\sim 1, \sim i})$. Hence,

$$\begin{aligned} u_i b_{n+1,i} &= z_i (-1)^i \det(A_{\sim 1, \sim i}) b_{n+1,i} = \underbrace{b_{n+1,i} z_i}_{=w \text{ (by (3.3))}} (-1)^i \det(A_{\sim 1, \sim i}) \\ &= w \cdot (-1)^i \det(A_{\sim 1, \sim i}). \end{aligned}$$

Hence, Equation (3.8) is proven in both cases. □

Now, (3.7) becomes

$$\begin{aligned} \Delta B^T e_{n+1} &= (u_1 b_{n+1,1}, u_2 b_{n+1,2}, \dots, u_{n+1} b_{n+1,n+1})^T \\ &= \left(w \cdot (-1)^1 \det(A_{\sim 1, \sim 1}), w \cdot (-1)^2 \det(A_{\sim 1, \sim 2}), \dots, \right. \\ &\quad \left. w \cdot (-1)^{n+1} \det(A_{\sim 1, \sim (n+1)}) \right)^T \quad (\text{by (3.8)}) \\ &= w \cdot \underbrace{\left((-1)^1 \det(A_{\sim 1, \sim 1}), (-1)^2 \det(A_{\sim 1, \sim 2}), \dots, (-1)^{n+1} \det(A_{\sim 1, \sim (n+1)}) \right)^T}_{= \mathbf{x} \quad (\text{by the definition of } \mathbf{x})} \\ &= w \mathbf{x}. \end{aligned}$$

Hence,

$$\begin{aligned} A \Delta B^T e_{n+1} &= A w \mathbf{x} = w \cdot \overbrace{A \mathbf{x}}^{= - \det A \cdot e_1 \quad (\text{by (3.6)})} \\ &= -w \cdot \underbrace{\det A}_{= a_{n+1, n+1} \cdot \det \bar{A}} \cdot e_1 \quad (\text{by (3.2)}) \\ &= -w \cdot a_{n+1, n+1} \cdot \underbrace{\det \bar{A}}_{= 0 \quad (\text{since we are in } \mathbb{M})} \cdot e_1 = 0. \end{aligned}$$

In other words, the $(n + 1)$ -st column of the matrix $A \Delta B^T$ is 0 (since the $(n + 1)$ -st column of the matrix $A \Delta B^T$ is $A \Delta B^T e_{n+1}$ (by (3.5), applied to $C = A \Delta B^T$ and $j = n + 1$)).

Now, fix $I \in P_k$. Then, the last column of the matrix $\text{sub}_{I+}^{I+}(A \Delta B^T)$ is 0 (because this column is a piece of the $(n + 1)$ -st column of the matrix $A \Delta B^T$, but as we have just shown the latter column is 0). Thus, $\det(\text{sub}_{I+}^{I+}(A \Delta B^T)) = 0$.

But Lemma 3.8 (applied to \mathbb{M} , $n + 1$, $n + 1$, $n + 1$, ΔB^T , $k + 1$, $I+$ and $I+$ instead of \mathbb{K} , n , m , p , B , k , P and Q) yields

$$\det(\text{sub}_{I+}^{I+}(A \Delta B^T)) = \sum_{\substack{R \subseteq [n+1]; \\ |R|=k+1}} \det(\text{sub}_{I+}^R A) \det(\text{sub}_R^{I+}(\Delta B^T)).$$

Comparing this with $\det(\text{sub}_{I+}^{I+}(A \Delta B^T)) = 0$, we obtain

$$0 = \sum_{\substack{R \subseteq [n+1]; \\ |R|=k+1}} \det(\text{sub}_{I+}^R A) \det(\text{sub}_R^{I+}(\Delta B^T)).$$

In the sum on the right hand side, all addends for which $n + 1 \notin R$ are zero (because if $R \subseteq [n + 1]$ satisfies $|R| = k + 1$ and $n + 1 \notin R$, then the last row of the matrix $\text{sub}_{I+}^R A$ consists of zeroes (by (3.1), since $n + 1 \notin R$ but $n + 1 \in I+$), and therefore we have $\det(\text{sub}_{I+}^R A) = 0$), and thus can be discarded. Hence, we are left with

$$0 = \sum_{\substack{R \subseteq [n+1]; \\ |R|=k+1; \\ n+1 \in R}} \det(\text{sub}_{I+}^R A) \det(\text{sub}_R^{I+}(\Delta B^T)).$$

But the subsets R of $[n + 1]$ satisfying $|R| = k + 1$ and $n + 1 \in R$ can be parametrized as $J+$ with J ranging over P_k . Hence, this rewrites further as

$$0 = \sum_{J \in P_k} \det(\text{sub}_{I+}^{J+} A) \det(\text{sub}_{J+}^{I+}(\Delta B^T)).$$

It is easily seen that $\det(\text{sub}_{J+}^{I+}(\Delta B^T)) = \det(\text{sub}_{I+}^{J+} B)u_J$ for each $J \in P_k$ (indeed, recall the definition of Δ and the fact that $u_{n+1} = 1$ and that $\det(C^T) = \det C$ for each square matrix C). Thus, the above equality simplifies to

$$0 = \sum_{J \in P_k} \det(\text{sub}_{I+}^{J+} A) \det(\text{sub}_{I+}^{J+} B)u_J.$$

Now, forget that we fixed I . We thus have proven that

$$0 = \sum_{J \in P_k} \det(\text{sub}_{I+}^{J+} A) \det(\text{sub}_{I+}^{J+} B)u_J \tag{3.9}$$

for each $I \in P_k$. This rewrites as $W\mathbf{u} = 0$ (indeed, the left hand side of (3.9) is the I -th entry of the zero vector 0 , whereas the right hand side of (3.9) is the I -th entry of $W\mathbf{u}$).

Now, consider the matrix W as a matrix in $\mathbb{M}^{P_k \times P_k}$. Then, Proposition 3.7 (applied to $P = P_k$) yields $\det W = 0$ in \mathbb{M} (since $\mathbf{u} \neq 0$ and $W\mathbf{u} = 0$). In view of the definition of \mathbb{M} , this rewrites as $\det \bar{A} \mid \det W$ in \mathbb{K} .

Let us consider the matrix W again as a matrix over \mathbb{K} . Each entry of W has the form $\det(\text{sub}_{I+}^{J+} A) \det(\text{sub}_{I+}^{J+} B)$ for some $I, J \in P_k$.

Claim 3. $\det(\text{sub}_{I+}^{J+} A)$ is a multiple of $a_{n+1, n+1}$ for all $I, J \in P_k$.

Proof of Claim 3. Let $I, J \in P_k$. Then, the equality (3.1) shows that the last row of the matrix $\text{sub}_{I+}^{J+} A$ is $(0, 0, \dots, 0, a_{n+1, n+1})$. Hence, an application of [4, Theorem 6.43] shows that $\det(\text{sub}_{I+}^{J+} A) = a_{n+1, n+1} \det(\text{sub}_I^J A)$. Thus, $\det(\text{sub}_{I+}^{J+} A)$ is a multiple of $a_{n+1, n+1}$. \square

By Claim 3, all entries of W are multiples of $a_{n+1, n+1}$. Hence, the determinant of W is a multiple of $(a_{n+1, n+1})^{|P_k|}$, thus a multiple of $a_{n+1, n+1}$ (since $|P_k| \geq 1$). In other words, $a_{n+1, n+1} \mid \det W$ in \mathbb{K} .

Recall that \mathbb{K} is a UFD. Also, the two polynomials $a_{n+1, n+1}$ and $\det \bar{A}$ in \mathbb{K} both have content 1, and don't have any indeterminates in common; thus, these two polynomials are coprime (by Proposition 3.4). Hence, any polynomial in \mathbb{K} that is divisible by both $a_{n+1, n+1}$ and $\det \bar{A}$ must be divisible by the product $a_{n+1, n+1} \cdot \det \bar{A}$ as well. Thus, from $a_{n+1, n+1} \mid \det W$ and $\det \bar{A} \mid \det W$, we obtain $a_{n+1, n+1} \cdot \det \bar{A} \mid \det W$. In view of (3.2), this rewrites as $\det A \mid \det W$. This proves Lemma 3.9. \square

We shall now derive Theorem 2.2 from Lemma 3.9, following the same idea as in [12, §2.7] and [13, Teorema 2.9.1] and [10]:

Proof of Theorem 2.1. We WLOG assume that $n > 0$ (otherwise, the result follows from $\det W = \det(0) = 0$).

We WLOG assume that \mathbb{K} is the polynomial ring over \mathbb{Z} in $(n + 1)^2 + ((n + 1)^2 - 1)$ indeterminates

$$\begin{aligned} a_{i,j} & \text{ for all } i \in [n + 1] \text{ and } j \in [n + 1]; \\ b_{i,j} & \text{ for all } i \in [n + 1] \text{ and } j \in [n + 1] \text{ except for } b_{n+1,n+1}. \end{aligned}$$

And, of course, we assume that the entries of A and B that are not zero by assumption are these indeterminates. Proposition 3.1 shows that the ring \mathbb{K} is a UFD (since it is a polynomial ring over \mathbb{Z}).

Let S be the multiplicative subset $\{a_{n+1,n+1}^p \mid p \in \mathbb{N}\}$ of \mathbb{K} . Then, all elements of S are regular (since they are monomials in a polynomial ring).

Let \mathbb{L} be the localization of the commutative ring \mathbb{K} at the multiplicative subset S . Then, Proposition 3.6(a) shows that the canonical ring homomorphism from \mathbb{K} to \mathbb{L} is injective; we shall thus consider it as an embedding. Also, Proposition 3.6(b) shows that \mathbb{L} is an integral domain.

Claim 1. *We claim that*

$$\det A \mid \det W \text{ in } \mathbb{L}. \tag{3.10}$$

Proof of Claim 1. Consider A, B and W as matrices over \mathbb{L} . The entry $a_{n+1,n+1}$ of A is invertible in \mathbb{L} (by the construction of \mathbb{L}). Hence, we can subtract appropriate scalar multiples⁷ of the $(n + 1)$ -st column of A from each other column of A to ensure that all entries of the last row of A become 0, except for $a_{n+1,n+1}$. (Specifically, for each $j \in [n]$, we have to subtract $a_{j,n+1}/a_{n+1,n+1}$ times the $(n + 1)$ -st column of A from the j -th column of A .) All these column transformations preserve the determinant $\det A$, and also preserve the minors $\det(\text{sub}_{I+}^{J+} A)$ for all $I, J \in P_k$ (because when the $(n + 1)$ -st column of A is subtracted from another column of A , the matrix $\text{sub}_{I+}^{J+} A$ either stays the same or undergoes an analogous column transformation⁸, which preserves its determinant); thus, they preserve the matrix W . Hence, we can replace A by the result of these transformations. This new matrix A satisfies (3.1). Hence, Lemma 3.9 (applied to \mathbb{L} instead of \mathbb{K}) yields that $\det A \mid \det W$ in \mathbb{L} . This proves (3.10). \square

But we must prove that $\det A \mid \det W$ in \mathbb{K} . Fortunately, this is easy: Since \mathbb{K} embeds into \mathbb{L} , we can translate our result “ $\det A \mid \det W$ in \mathbb{L} ” as “ $\det A \mid a_{n+1,n+1}^p \det W$ in \mathbb{K} for an appropriate $p \in \mathbb{N}$ ” (by Proposition 3.6(c), applied to $a = \det A$ and $b = \det W$). Consider this p .

Claim 2. *The polynomial $a_{n+1,n+1} \in \mathbb{K}$ is coprime to $\det A$.*

Proof of Claim 2. The polynomial $\det A$ contains the monomial $a_{1,n+1}a_{2,n} \cdots a_{n+1,1} = \prod_{i \in [n+1]} a_{i,n+2-i}$, and thus is not a multiple of $a_{n+1,n+1}$. Hence, it is coprime to $a_{n+1,n+1}$ (since the only non-unit divisor of $a_{n+1,n+1}$ is $a_{n+1,n+1}$ itself, up to scaling by units). \square

So we know that $a_{n+1,n+1}$ is coprime to $\det A$. Hence, its power $a_{n+1,n+1}^p$ is coprime to $\det A$ as well. Hence, we can cancel the $a_{n+1,n+1}^p$ from the divisibility $\det A \mid a_{n+1,n+1}^p \det W$, and conclude that $\det A \mid \det W$ in \mathbb{K} . This proves Theorem 2.1. \square

⁷The scalars, of course, come from \mathbb{L} here.

⁸Here we are using the fact that $n + 1 \in J+$ (so that the matrix $\text{sub}_{I+}^{J+} A$ contains part of the $(n + 1)$ -st column of A).

Proof of Theorem 2.2. We WLOG assume that \mathbb{K} is the polynomial ring over \mathbb{Z} in the $((n+1)^2 - 1) + ((n+1)^2 - 1)$ indeterminates

$$\begin{aligned} a_{i,j} & \text{ for all } i \in [n+1] \text{ and } j \in [n+1] \text{ except for } a_{n+1,n+1}; \\ b_{i,j} & \text{ for all } i \in [n+1] \text{ and } j \in [n+1] \text{ except for } b_{n+1,n+1}. \end{aligned}$$

And, of course, we assume that the entries of A and B that are not zero by assumption are these indeterminates. The ring \mathbb{K} is a UFD (by Proposition 3.1).

WLOG assume that $n > 0$ (otherwise, the result follows from $\det W = \det(0) = 0$). Thus, the monomial $a_{1,n+1}a_{2,n} \cdots a_{n+1,1} = \prod_{i \in [n+1]} a_{i,n+2-i}$ occurs in the polynomial $\det A$ with coefficient ± 1 . Hence, the polynomial $\det A$ has content 1. Similarly, the polynomial $\det B$ has content 1.

Theorem 2.1 yields $\det A \mid \det W$. The same argument yields $\det B \mid \det W$ (since the matrices A and B play symmetric roles in the construction of W). But Proposition 3.4 shows that the polynomials $\det A$ and $\det B$ in \mathbb{K} are coprime (because they have content 1, and don't have any indeterminates in common). Thus, any polynomial in \mathbb{K} that is divisible by both $\det A$ and $\det B$ must be divisible by the product $(\det A)(\det B)$ as well. Thus, from $\det A \mid \det W$ and $\det B \mid \det W$, we obtain $(\det A)(\det B) \mid \det W$. This proves Theorem 2.2. \square

4 Further questions


While Theorems 2.1 and 2.2 are now proven, the field appears far from fully harvested. Three questions readily emerge:

Question 4.1. What can be said about $\frac{\det W}{\det A}$ (in Theorem 2.1) and $\frac{\det W}{(\det A)(\det B)}$ (in Theorem 2.2)? Are there formulas?

Question 4.2. Are there more direct proofs of Theorems 2.1 and 2.2, avoiding the use of polynomial rings and their properties and instead “staying inside \mathbb{K} ”? Such proofs might help answer the previous question.

Question 4.3. The entries of our matrix W were products of minors of two $(n+1) \times (n+1)$ -matrices that each use the last row and the last column. What can be said about products of minors of two $(n+m) \times (n+m)$ -matrices that each use the last m rows and the last m columns, where m is an arbitrary positive integer? The “Generalized Sylvester’s identity” in [12, §2.7] answers this for the case of one matrix. It is not quite obvious what the right analogues of the conditions $a_{n+1,n+1} = 0$ and $b_{n+1,n+1} = 0$ are; furthermore, nontrivial examples become even more computationally challenging.

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Boundary-type sets of strong product of directed graphs*

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Abstract

Let $D = (V, E)$ be a strongly connected digraph and let u and v be two vertices in D . The maximum distance $md(u, v)$ is defined as $md(u, v) = \max\{\vec{d}(u, v), \vec{d}(v, u)\}$, where $\vec{d}(u, v)$ denotes the length of a shortest directed u - v path in D . This is a metric. The boundary, contour, eccentricity and periphery sets of a strongly connected digraph D with respect to this metric have been defined. The boundary-type sets of the strong product of two digraphs is investigated in this article.

Keywords: Maximum distance, boundary-type sets, strongly connected digraph, strong product.

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1 Introduction

Directed graphs or in short digraphs have immense applications in almost all areas of science and even in sociology. A directed network is a network in which each edge has a direction, pointing from one vertex to another. They can be represented as directed graphs.

Road traffic networks are the most frequently met examples of one-way networks. A two-way street is one in which vehicles are allowed to travel in both directions. The advantages of a one-way street network over a two-way street pattern are discussed in [14]. But when one-way traffic is introduced in a two-way network, the distance between places in one of the directions may increase. So the problem of designing a network is to minimize the distance between places and the cost of construction.

The one-way problem was first studied by Robbins [13]. It finds applications in various fields like computer science, biology, etc. In [2], directed graphs are used to analyze the local properties of internet connectivity. Neurons are connected in intricate communication networks established during development to convey sensory information from peripheral receptors of sensory neurons to the central nervous system and to convey commands from the central nervous system to effector organs [12].

The boundary-type sets of a graph, the *boundary*, *contour*, *eccentricity*, and *periphery sets* of a graph were studied in [5] and [7]. It is very difficult to identify the various boundary-type sets in large networks. So we try to decompose the network into smaller networks and identify the boundary-type sets. The four standard graph products, namely Cartesian, direct, strong, and lexicographic products can be extended to digraphs as well. Marc Hellmuth and Tilen Marc developed a polynomial-time algorithm for determining the prime factor decomposition of strong product of digraphs [11].

The directed distance defined in digraphs is generally not a metric. As we are concerned with the problem of designing the network to minimize the distance between places at a minimum cost, we consider the distance *maximum distance* or in short, *m-distance* which is a metric that was introduced by Chartrand and Tian in [8]. It gives the maximum of the directed distances in either direction and is denoted by $md(u, v)$. So minimizing $md(u, v)$ results in minimizing the distance between the nodes in both directions. An undirected graph G can be identified as a symmetric digraph, that is, one for which $(u, v) \in E(G)$ if and only if $(v, u) \in E(G)$, and the metric md is the usual distance metric in undirected graphs.

The boundary-type sets of the Cartesian product of two digraphs were studied in [6]. In this paper, a similar study is conducted for the strong product of digraphs.

2 Preliminaries

A *directed graph* or a *digraph* D consists of a non-empty finite set $V(D)$ of elements called vertices and a finite set $E(D)$ of ordered pairs of distinct vertices called arcs or edges [1]. We call $V(D)$ the vertex set and $E(D)$ the edge set of D . We write $D = (V, E)$ to denote the digraph D with vertex set V and edge set E . For an edge (u, v) , the first vertex u of the ordered pair is the tail of the edge and the second vertex v is the head; together they are the endpoints. This definition of a digraph does not allow loops (edges whose head and tail coincide) or parallel edges (pairs of edges with the same tail and the same head). The underlying graph UD of a digraph D is the simple graph with the vertex set $V(D)$ and the unordered pair $(x, y) \in E(UD)$ if and only if either $(x, y) \in E(D)$ or $(y, x) \in E(D)$.

The following concepts are taken from [1].

For a vertex v in a digraph $D = (V, E)$, the neighborhoods are defined as follows:

$$N_D^+(v) = \{w \in V : (v, w) \in E\}, \quad N_D^-(v) = \{u \in V : (u, v) \in E\}.$$

The sets $N_D^+(v)$, $N_D^-(v)$, and $N_D(v) = N_D^+(v) \cup N_D^-(v)$ are called the out-neighborhood, in-neighborhood, and neighborhood of v . These neighborhoods are called open neighborhoods of v . Similarly, we can define closed neighborhoods of v (neighbors including v). The closed neighborhood of v is denoted by $N_D[v]$. That is, $N_D[v] = N_D(v) \cup \{v\}$.

A *directed path* is a directed graph with $V(P) \neq \emptyset$ with distinct vertices u_1, u_2, \dots, u_k and edges e_1, e_2, \dots, e_{k-1} such that e_i is an edge directed from u_i to u_{i+1} for $1 \leq i \leq k - 1$. In this article, a path will always mean a ‘directed path’. A digraph is *strongly connected* or *strong* if, for each ordered pair (u, v) of vertices, there is a path from u to v . A digraph is *weakly connected* if its underlying graph is connected. A *strong component* of a digraph D is a maximal induced subdigraph of D which is strong. If D_1, D_2, \dots, D_t are the strong components of D , then $V(D_1) \cup V(D_2) \cup \dots \cup V(D_t) = V(D)$ and $V(D_i) \cap V(D_j) = \emptyset$ for every $i \neq j$.

The *length* of a path is the number of edges in the path. The *directed distance* $\vec{d}(u, v)$ between two vertices $u, v \in V(D)$ is the length of the shortest directed path from u to v , or infinity if no such path exists. Note that this distance is not a metric, as generally $\vec{d}(u, v) \neq \vec{d}(v, u)$.

So in [8], Chartrand and Tian introduced two other distances between the vertices u and v in a strong digraph, namely the maximum distance $md(u, v) = \max\{\vec{d}(u, v), \vec{d}(v, u)\}$ and the sum distance $sd(u, v) = \vec{d}(u, v) + \vec{d}(v, u)$, both of which are metrics. In this article, we deal with the maximum distance, md .

Remark 2.1. $md(u, v)$ is denoted by $d(u, v)$ hereafter.

The *m-eccentricity* of a vertex v , the *m-radius* and the *m-diameter* of a digraph D are also defined in [8]. Consistent with our notation $d(u, v)$ for maximum distance between the vertices u and v , we denote them respectively as $\text{ecc}(v)$, $\text{rad}(D)$, and $\text{diam}(D)$. Thus, $\text{ecc}(v) = \max_{u \in V(D)} d(v, u)$, $\text{rad}(D) = \min_{v \in V(D)} \text{ecc}(v)$, and $\text{diam}(D) = \max_{v \in V(D)} \text{ecc}(v)$, where $\text{ecc}(v)$ denotes *m-eccentricity* of v .

If a digraph D is strongly connected, then the maximum distance between every pair of vertices is finite, and hence the *m-eccentricity* of every vertex in D is finite. Otherwise, D has more than one strong component, and the maximum distance between two vertices lying in different strong components of D is infinity. So if D is not strongly connected, then the *m-eccentricity* of every vertex in D is infinity.

2.1 Definitions of boundary-type sets

We define the boundary-type sets of a digraph D with respect to the metric maximum distance. Most of the following definitions are analogous to the definitions in [7]. Let D be a strong digraph and $u, v \in V(D)$. The vertex v is said to be a *boundary vertex* of u if no neighbor of v is further away from u than v . Hereafter, we denote $N_D(v)$ and $N_D[v]$ by $N(v)$ and $N[v]$, respectively.

A vertex v is called a *boundary vertex* of D if it is the boundary vertex of some vertex $u \in V(D)$.

Definition 2.2. The *boundary* $\partial(D)$ of D is the set of all of its boundary vertices

$$\partial(D) = \{v \in V(D) : \exists u \in V(D) \text{ such that } \forall w \in N(v), d(u, w) \leq d(u, v)\}.$$

Given $u, v \in V(D)$, the vertex v is called an *eccentric vertex* of u if no vertex in $V(D)$ is further away from u than v ; that is, if $d(u, v) = \text{ecc}(u)$. A vertex v is called an *eccentric vertex* of digraph D if it is the eccentric vertex of some vertex $u \in V(D)$.

Definition 2.3. The *eccentricity* $\text{Ecc}(D)$ of a digraph D is the set of all of its eccentric vertices

$$\text{Ecc}(D) = \{v \in V(D) : \exists u \in V(D) \text{ such that } \text{ecc}(u) = d(u, v)\}.$$

In a similar way, we can define the *eccentricity* of any proper subset W of the vertex set $V(D)$:

$$\text{Ecc}(W) = \{v \in V(D) : \exists u \in W \text{ such that } \text{ecc}(u) = d(u, v)\}.$$

A vertex $v \in V(D)$ is called a *peripheral vertex* of D if no vertex in $V(D)$ has an eccentricity greater than $\text{ecc}(v)$; that is, if the eccentricity of v is equal to the diameter $\text{diam}(D)$ of D .

Definition 2.4. The *periphery* $\text{Per}(D)$ of a digraph D is the set of all of its peripheral vertices

$$\begin{aligned} \text{Per}(D) &= \{v \in V(D) : \text{ecc}(u) \leq \text{ecc}(v), \forall u \in V(D)\} \\ &= \{v \in V(D) : \text{ecc}(v) = \text{diam}(D)\}. \end{aligned}$$

A vertex $v \in V(D)$ is called a *contour vertex* of digraph D if no neighbor vertex of v has an eccentricity greater than $\text{ecc}(v)$. The following definition is from [5].

Definition 2.5. The *contour* $\text{Ct}(D)$ of a digraph D is the set of all of its contour vertices

$$\text{Ct}(D) = \{v \in V(D) : \text{ecc}(u) \leq \text{ecc}(v), \forall u \in N(v)\}.$$

As in the case of undirected graphs [3] we have,

1. $\text{Per}(D) \subseteq \text{Ct}(D) \cap \text{Ecc}(D)$,
2. $\text{Ecc}(D) \cup \text{Ct}(D) \subseteq \partial(D)$.

This is because a peripheral vertex is a vertex having the maximum eccentricity in the digraph D and so every peripheral vertex in D is a contour vertex in D as well as the eccentric vertex of a diametrical vertex in D .

If v is an eccentric vertex of a vertex u , then v is a boundary vertex of u . Also if v is a contour vertex, then $\text{ecc}(u) \leq \text{ecc}(v)$ for all $u \in N(v)$. So there exists some vertex $w \in V(D)$ such that $d(w, u) \leq d(w, v)$ for all $u \in N(v)$, and hence v is a boundary vertex of w .

The open neighborhood $N(v)$ can be replaced by the closed neighborhood $N[v]$ in the definitions of the boundary and the contour sets. This does not affect the definitions and is necessary for proving the relationship between the boundary and the contour sets of the strong product of two digraphs and its factors.

3 Strong product of directed graphs

The strong product $D_1 \boxtimes D_2$ of two digraphs D_1 and D_2 with vertex sets $V(D_1) = \{u_1, u_2, \dots, u_m\}$ and $V(D_2) = \{v_1, v_2, \dots, v_n\}$ is the digraph having the vertex set $V(D_1) \times V(D_2)$ and with arc set $E(D_1 \boxtimes D_2)$ defined as follows. A vertex (u_i, v_r) is adjacent to (u_j, v_s) in $D_1 \boxtimes D_2$ if either

1. $(u_i, u_j) \in E(D_1), v_r = v_s$, or
2. $u_i = u_j, (v_r, v_s) \in E(D_2)$, or
3. $(u_i, u_j) \in E(D_1), (v_r, v_s) \in E(D_2)$.

The strong product of digraphs is commutative [10]. The distance between two vertices (g, h) and (g', h') in the strong product $G \boxtimes H$ of two graphs G and H is given in [9] as follows:

$$d_{G \boxtimes H}((g, h), (g', h')) = \max\{d_G(g, g'), d_H(h, h')\}.$$

So in the case of two digraphs D_1 and D_2 , it follows that the directed distance

$$\vec{d}_{D_1 \boxtimes D_2}((u_i, v_r), (u_j, v_s)) = \max\{\vec{d}_{D_1}(u_i, u_j), \vec{d}_{D_2}(v_r, v_s)\}.$$

Lemma 3.1. *Let D_1 and D_2 be two strongly connected digraphs. Then*

$$\begin{aligned} d_{D_1 \boxtimes D_2}((u_i, v_r), (u_j, v_s)) &= \max\{d_{D_1}(u_i, u_j), d_{D_2}(v_r, v_s)\}, \\ \text{ecc}_{D_1 \boxtimes D_2}(u_i, v_r) &= \max\{\text{ecc}_{D_1}(u_i), \text{ecc}_{D_2}(v_r)\}. \end{aligned}$$

Proof.

$$\begin{aligned} d_{D_1 \boxtimes D_2}((u_i, v_r), (u_j, v_s)) &= \max\{\vec{d}_{D_1 \boxtimes D_2}((u_i, v_r), (u_j, v_s)), \vec{d}_{D_1 \boxtimes D_2}((u_j, v_s), (u_i, v_r))\} \\ &= \max\{\max\{\vec{d}_{D_1}(u_i, u_j), \vec{d}_{D_2}(v_r, v_s)\}, \max\{\vec{d}_{D_1}(u_j, u_i), \vec{d}_{D_2}(v_s, v_r)\}\} \\ &= \max\{\max\{\vec{d}_{D_1}(u_i, u_j), \vec{d}_{D_2}(v_r, v_s), \vec{d}_{D_1}(u_j, u_i), \vec{d}_{D_2}(v_s, v_r)\}\} \\ &= \max\{\max\{\vec{d}_{D_1}(u_i, u_j), \vec{d}_{D_1}(u_j, u_i)\}, \max\{\vec{d}_{D_2}(v_r, v_s), \vec{d}_{D_2}(v_s, v_r)\}\} \\ &= \max\{d_{D_1}(u_i, u_j), d_{D_2}(v_r, v_s)\}. \end{aligned}$$

Hence it follows that

$$\begin{aligned} \text{ecc}_{D_1 \boxtimes D_2}(u_i, v_r) &= \max\{d_{D_1 \boxtimes D_2}((u_i, v_r), (u_j, v_s)) : (u_j, v_s) \in V(D_1 \boxtimes D_2)\} \\ &= \max\{\max\{d_{D_1}(u_i, u_j), d_{D_2}(v_r, v_s)\} : u_j \in V(D_1), v_s \in V(D_2)\} \\ &= \max\{\max\{d_{D_1}(u_i, u_j) : u_j \in V(D_1)\}, \max\{d_{D_2}(v_r, v_s) : v_s \in V(D_2)\}\} \\ &= \max\{\text{ecc}_{D_1}(u_i), \text{ecc}_{D_2}(v_r)\}. \quad \square \end{aligned}$$

Corollary 3.2. *Let D_1 and D_2 be two strongly connected digraphs. Then*

$$\begin{aligned} \text{rad}(D_1 \boxtimes D_2) &= \max\{\text{rad}(D_1), \text{rad}(D_2)\}, \\ \text{diam}(D_1 \boxtimes D_2) &= \max\{\text{diam}(D_1), \text{diam}(D_2)\}. \end{aligned}$$

Proof.

$$\begin{aligned}
 \text{rad}(D_1 \boxtimes D_2) &= \min_{(u_i, v_r) \in V(D_1 \boxtimes D_2)} \text{ecc}(u_i, v_r) \\
 &= \min_{\substack{u_i \in V(D_1) \\ v_r \in V(D_2)}} \max\{\text{ecc}_{D_1}(u_i), \text{ecc}_{D_2}(v_r)\} \\
 &= \max\left\{ \min_{u_i \in V(D_1)} \text{ecc}(u_i), \min_{v_r \in V(D_2)} \text{ecc}(v_r) \right\} \\
 &= \max\{\text{rad}(D_1), \text{rad}(D_2)\}, \\
 \\
 \text{diam}(D_1 \boxtimes D_2) &= \max_{(u_i, v_r) \in V(D_1 \boxtimes D_2)} \text{ecc}(u_i, v_r) \\
 &= \max_{\substack{u_i \in V(D_1) \\ v_r \in V(D_2)}} \max\{\text{ecc}_{D_1}(u_i), \text{ecc}_{D_2}(v_r)\} \\
 &= \max\left\{ \max_{u_i \in V(D_1)} \text{ecc}(u_i), \max_{v_r \in V(D_2)} \text{ecc}(v_r) \right\} \\
 &= \max\{\text{diam}(D_1), \text{diam}(D_2)\}. \quad \square
 \end{aligned}$$

The strong product of two directed graphs is strongly connected if and only if both the digraphs are strongly connected [9]. Also if G and H are two undirected graphs, $N_{G \boxtimes H}[(g, h)] = N_G[g] \times N_H[h]$ [9]. Since the neighbors of a vertex in a directed graph are exactly its neighbors in the underlying graph, it follows that

$$N_{D_1 \boxtimes D_2}[(u_i, v_r)] = N_{G \boxtimes H}[(u_i, v_r)] = N_G[u_i] \times N_H[v_r] = N_{D_1}[u_i] \times N_{D_2}[v_r],$$

where G and H are the underlying graphs of D_1 and D_2 , respectively. In [4], Cáceres et al. presented a description of the boundary-type sets of two undirected graphs and the description of the boundary is as follows.

For two graphs G and H , $\partial(G \boxtimes H) = (\partial(G) \times V(H)) \cup (V(G) \times \partial(H))$. But this result does not hold in the case of directed graphs.

Consider the strong product, $D_1 \boxtimes D_2$ of the digraphs D_1 and D_2 in Figure 1. The eccentricity of each vertex is displayed near the vertex in red color.

$$\begin{aligned}
 \text{Per}(D_1) &= \text{Ecc}(D_1) = \text{Ct}(D_1) = \{u_1, u_4\}, \\
 \text{Per}(D_2) &= \text{Ecc}(D_2) = \text{Ct}(D_2) = \{v_1, v_2\}, \text{ and} \\
 \text{Per}(D_1 \boxtimes D_2) &= \text{Ecc}(D_1 \boxtimes D_2) = \text{Ct}(D_1 \boxtimes D_2) \\
 &= \{(u_1, v_1), (u_4, v_1), (u_1, v_2), (u_4, v_2)\}.
 \end{aligned}$$

$$\begin{aligned}
 \partial(D_1) &= \{u_1, u_4\}, \\
 \partial(D_2) &= \{v_1, v_2\}, \text{ and} \\
 \partial(D_1 \boxtimes D_2) &= \{(u_1, v_1), (u_4, v_1), (u_1, v_2), (u_4, v_2)\}.
 \end{aligned}$$

The reason for $(u_2, v_1), (u_2, v_2), (u_3, v_1), (u_3, v_2) \notin \partial(D_1 \boxtimes D_2)$ is explained after the proof of Theorem 3.3.

Now we present the results concerning the boundary-type sets of the strong product of two strongly connected digraphs. In all these results, D_1 and D_2 can be interchanged due to the commutativity of strong product of digraphs.

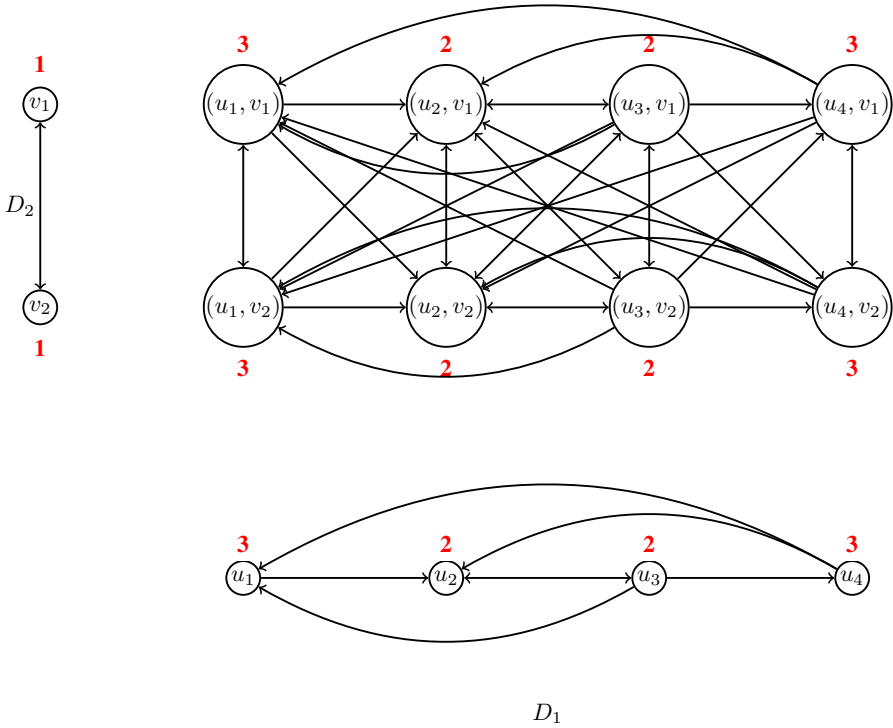


Figure 1: $D_1 \boxtimes D_2$.

We have, $\partial(D_1 \boxtimes D_2) \subseteq [\partial(D_1) \times V(D_2)] \cup [V(D_1) \times \partial(D_2)]$.

To this end, let $(u_i, v_r) \in \partial(D_1 \boxtimes D_2)$. Then there exists a vertex $(u_j, v_s) \in V(D_1 \boxtimes D_2)$ such that $d((u_j, v_s), (u_i, v_r)) \geq d((u_j, v_s), (u_k, v_q))$ for every $(u_k, v_q) \in N[(u_i, v_r)]$. This implies, $\max\{d(u_j, u_i), d(v_s, v_r)\} \geq \max\{d(u_j, u_k), d(v_s, v_q)\}$ for every $u_k \in N[u_i]$ and for every $v_q \in N[v_r]$. Hence $d(u_j, u_i) \geq d(u_j, u_k)$ for every $u_k \in N[u_i]$, or $d(v_s, v_r) \geq d(v_s, v_q)$ for every $v_q \in N[v_r]$. Thus, $u_i \in \partial(D_1)$ or $v_r \in \partial(D_2)$ or both. That is, if $(u_i, v_r) \in \partial(D_1 \boxtimes D_2)$, then at least one of the vertices u_i and v_r must be a boundary vertex in the corresponding factor graph.

Theorem 3.3. Let D_1 and D_2 be two strongly connected digraphs. Then $\partial(D_1 \boxtimes D_2) = A_1 \cup A_2 \cup A_3$, where

$$A_1 = \partial(D_1) \times \partial(D_2),$$

$$A_2 = \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \partial(D_1), v_r \notin \partial(D_2), \text{ and} \\ \exists v_t \in V(D_2) \text{ such that } d(v_t, v_q) \leq \text{ecc}(u_i), \forall v_q \in N[v_r]\},$$

$$A_3 = \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \notin \partial(D_1), v_r \in \partial(D_2), \text{ and} \\ \exists u_\ell \in V(D_1) \text{ such that } d(u_\ell, u_k) \leq \text{ecc}(v_r), \forall u_k \in N[u_i]\}.$$

Proof. Suppose that $(u_i, v_r) \in \partial(D_1 \boxtimes D_2)$.

Then there exists a vertex $(u_j, v_s) \in V(D_1 \boxtimes D_2)$ such that $d((u_j, v_s), (u_i, v_r)) \geq d((u_j, v_s), (u_k, v_q))$ for all vertices $(u_k, v_q) \in N[(u_i, v_r)]$. Since $d((u_j, v_s), (u_i, v_r)) = \max\{d(u_j, u_i), d(v_s, v_r)\}$ and $d((u_j, v_s), (u_k, v_q)) = \max\{d(u_j, u_k), d(v_s, v_q)\}$, we get $\max\{d(u_j, u_i), d(v_s, v_r)\} \geq \max\{d(u_j, u_k), d(v_s, v_q)\}$ for all $u_k \in N[u_i], v_q \in N[v_r]$. We distinguish four cases:

1. $\max\{d(u_j, u_i), d(v_s, v_r)\} = d(u_j, u_i)$ and $d(v_s, v_r) \geq d(v_s, v_q)$ for all $v_q \in N[v_r]$;
2. $\max\{d(u_j, u_i), d(v_s, v_r)\} = d(u_j, u_i)$ and $d(v_s, v_r) \geq d(v_s, v_q)$ does not hold for all $v_q \in N[v_r]$;
3. $\max\{d(u_j, u_i), d(v_s, v_r)\} = d(v_s, v_r)$ and $d(u_j, u_i) \geq d(u_j, u_k)$ for all $u_k \in N[u_i]$;
4. $\max\{d(u_j, u_i), d(v_s, v_r)\} = d(v_s, v_r)$ and $d(u_j, u_i) \geq d(u_j, u_k)$ does not hold for all $u_k \in N[u_i]$.

In cases 1 and 3, $d(u_j, u_i) \geq d(u_j, u_k)$ for all $u_k \in N[u_i]$ and $d(v_s, v_r) \geq d(v_s, v_q)$ for all $v_q \in N[v_r]$. So $u_i \in \partial(D_1), v_r \in \partial(D_2)$, and hence $(u_i, v_r) \in A_1$.

In case 2, $u_i \in \partial(D_1)$ and v_r is not a boundary vertex of v_s in D_2 . If there exists any vertex v_t such that v_r is a boundary vertex of v_t , then we get $(u_i, v_r) \in A_1$. Otherwise, since $v_r \notin \partial(D_2)$, for every vertex $v_t \in V(D_2)$, there exists some vertex $v_q \in N[v_r]$ such that $d(v_t, v_r) < d(v_t, v_q)$. Hence if (u_i, v_r) is a boundary vertex of a vertex (u_ℓ, v_t) in $D_1 \boxtimes D_2$, then $d((u_\ell, v_t), (u_i, v_r)) = \max\{d(u_\ell, u_i), d(v_t, v_r)\} = d(u_\ell, u_i) > d(v_t, v_r)$, for otherwise $d(u_\ell, u_i) \leq d(v_t, v_r)$ and so we get $d((u_\ell, v_t), (u_i, v_r)) = d(v_t, v_r) < d(v_t, v_q) = d((u_\ell, v_t), (u_i, v_q))$, where $(u_i, v_q) \in N[(u_i, v_r)]$.

Let $(u_k, v_q) \in N[(u_i, v_r)]$. Then $d((u_\ell, v_t), (u_k, v_q)) = \max\{d(u_\ell, u_k), d(v_t, v_q)\}$. If (u_i, v_r) is a boundary vertex of (u_ℓ, v_t) , then $\max\{d(u_\ell, u_i), d(v_t, v_r)\} \geq \max\{d(u_\ell, u_k), d(v_t, v_q)\}$. So the necessary condition for the vertex (u_i, v_r) such that $u_i \in \partial(D_1)$ and $v_r \notin \partial(D_2)$ to be a boundary vertex of the vertex (u_ℓ, v_t) in $D_1 \boxtimes D_2$ is $d(u_\ell, u_i) \geq d(v_t, v_q)$ for all $v_q \in N[v_r]$. Since $\text{ecc}(u_i) \geq d(u_\ell, u_i)$ for all $u_\ell \in V(D_1)$, the necessary condition becomes $\text{ecc}(u_i) \geq d(v_t, v_q)$ for all $v_q \in N[v_r]$. Thus, $(u_i, v_r) \in A_2$.

Thus in case 2, $(u_i, v_r) \in A_1 \cup A_2$.

In case 4, $v_r \in \partial(D_2)$ and u_i is not a boundary vertex of u_j in D_1 . As in case 2, it follows that $(u_i, v_r) \in A_1 \cup A_3$.

Thus in all cases, we get $\partial(D_1 \boxtimes D_2) \subseteq A_1 \cup A_2 \cup A_3$.

Conversely, suppose that $(u_i, v_r) \in A_1 \cup A_2 \cup A_3$. First let $(u_i, v_r) \in A_1$. Then $u_i \in \partial(D_1)$ and $v_r \in \partial(D_2)$. So there exists vertices $u_j \in V(D_1), v_s \in V(D_2)$ such that $d(u_j, u_i) \geq d(u_j, u_k)$ for every $u_k \in N[u_i]$, and $d(v_s, v_r) \geq d(v_s, v_q)$ for every $v_q \in N[v_r]$. Hence in $D_1 \boxtimes D_2$, $d((u_j, v_s), (u_i, v_r)) = \max\{d(u_j, u_i), d(v_s, v_r)\} \geq \max\{d(u_j, u_k), d(v_s, v_q)\} = d((u_j, v_s), (u_k, v_q))$ for all vertices $(u_k, v_q) \in N[(u_i, v_r)]$. Thus, $A_1 \subseteq \partial(D_1 \boxtimes D_2)$.

Now let $(u_i, v_r) \in A_2$. Then $u_i \in \partial(D_1), v_r \notin \partial(D_2)$ and there exists some vertex $v_t \in V(D_2)$ such that $d(v_t, v_r) \leq \text{ecc}(u_i)$, for all $v_q \in N[v_r]$. Since $u_i \in \partial(D_1)$, there exists at least one vertex $u_j \in V(D_1)$ such that $d(u_j, u_i) \geq d(u_j, u_k)$ for every $u_k \in N[u_i]$. Of these vertices, let u_b be a vertex such that $d(u_b, u_i) = \text{ecc}(u_i)$. Hence in $D_1 \boxtimes D_2$,

$$\begin{aligned} d((u_b, v_t), (u_i, v_r)) &= \max\{d(u_b, u_i), d(v_t, v_r)\} \\ &\geq \max\{d(u_b, u_k), d(v_t, v_q)\} = d((u_b, v_t), (u_k, v_q)) \end{aligned}$$

for all $(u_k, v_q) \in N[(u_i, v_r)]$, since $d(v_t, v_q) \leq \text{ecc}(u_i) = d(u_b, u_i)$ for all $v_q \in N[v_r]$. Thus, (u_i, v_r) is a boundary vertex of (u_b, v_t) in $D_1 \boxtimes D_2$ and hence $A_2 \subseteq \partial(D_1 \boxtimes D_2)$.

By analogous arguments and since the strong product of digraphs is commutative, it follows that $A_3 \subseteq \partial(D_1 \boxtimes D_2)$.

Hence $A_1 \cup A_2 \cup A_3 \subseteq \partial(D_1 \boxtimes D_2)$. □

Now consider Figure 1. $\text{ecc}(v_1) = \text{ecc}(v_2) = 1$. $N[u_2] = N[u_3] = \{u_1, u_2, u_3, u_4\}$, $d(u_1, u_4) = 3$, $d(u_1, u_2) = d(u_1, u_3) = d(u_2, u_4) = d(u_3, u_4) = 2$, and $d(u_2, u_3) = 1$. $u_2 \notin \partial(D_1)$ and hence $(u_2, v_1), (u_2, v_2) \notin \partial(D_1 \boxtimes D_2)$, since there is no vertex $u_\ell \in V(D_1)$ such that $d(u_\ell, u_k) \leq 1$ for all $u_k \in N[u_2]$. For similar reasons, $(u_3, v_1), (u_3, v_2) \notin \partial(D_1 \boxtimes D_2)$.

Consider the strong product of two connected undirected graphs. In the case of an undirected graph, the *maximum distance* between two vertices is the usual distance between the vertices. Also, since we deal with the distance between any two distinct vertices, it doesn't matter whether the undirected graphs are simple or not; that is, whether they contain loops or parallel edges. So we state the result for any two connected nontrivial (not equal to K_1) undirected graphs.

Remark 3.4. The description for the boundary set of the strong product of two graphs (undirected graphs) G and H presented in [4] holds only for the product of two *nontrivial graphs* G and H . To this end, let $H = K_1 = (\{v\}, \emptyset)$. We have, $\partial(K_1) = \{v\}$ (since all vertices of a complete graph are boundary vertices of the graph), and hence $\partial(G) \hat{=} \partial(G \boxtimes K_1) = (\partial(G) \times \{v\}) \cup (V(G) \times \{v\}) \hat{=} V(G)$, which is not true in general.

Corollary 3.5. *Let D_1 and D_2 be two nontrivial connected undirected graphs. Then*

$$\partial(D_1 \boxtimes D_2) = [\partial(D_1) \times V(D_2)] \cup [V(D_1) \times \partial(D_2)].$$

Proof. By Theorem 3.3, if D_1 and D_2 are two strongly connected digraphs, $\partial(D_1 \boxtimes D_2) = A_1 \cup A_2 \cup A_3$. Since D_1 and D_2 are given to be two nontrivial undirected graphs, $\text{ecc}(u_i) \geq 1$ for all $u_i \in V(D_1)$, $\text{ecc}(v_r) \geq 1$ for all $v_r \in V(D_2)$, $d(u_i, u_k) = 1$ for all $u_k \in N(u_i)$, and $d(v_r, v_q) = 1$ for all $v_q \in N(v_r)$. Thus,

$$A_1 = \partial(D_1) \times \partial(D_2),$$

$$\begin{aligned} A_2 &= \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \partial(D_1), v_r \notin \partial(D_2), \text{ and} \\ &\quad \exists v_t \in V(D_2) \text{ such that } d(v_t, v_q) \leq \text{ecc}(u_i), \forall v_q \in N(v_r)\} \\ &= \partial(D_1) \times V(D_2), \end{aligned}$$

$$\begin{aligned} A_3 &= \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \notin \partial(D_1), v_r \in \partial(D_2), \text{ and} \\ &\quad \exists u_\ell \in V(D_1) \text{ such that } d(u_\ell, u_k) \leq \text{ecc}(v_r), \forall u_k \in N(u_i)\} \\ &= V(D_1) \times \partial(D_2). \end{aligned}$$

Therefore, $\partial(D_1 \boxtimes D_2) = A_1 \cup A_2 \cup A_3 = [\partial(D_1) \times V(D_2)] \cup [V(D_1) \times \partial(D_2)]$. □

Theorem 3.6. *Let D_1 and D_2 be two strongly connected digraphs.*

1. *If $\text{diam}(D_1) < \text{diam}(D_2)$, then $\text{Per}(D_1 \boxtimes D_2) = V(D_1) \times \text{Per}(D_2)$.*
2. *If $\text{diam}(D_1) = \text{diam}(D_2)$, then $\text{Per}(D_1 \boxtimes D_2) = [\text{Per}(D_1) \times V(D_2)] \cup [V(D_1) \times \text{Per}(D_2)]$.*

Proof.

1. Let $\text{diam}(D_2) = n$. Let $v_r \in \text{Per}(D_2)$.

Then for all $u_i \in V(D_1)$, $\text{ecc}(u_i, v_r) = \max\{\text{ecc}(u_i), \text{ecc}(v_r)\} = n$. Hence $(u_i, v_r) \in \text{Per}(D_1 \boxtimes D_2)$. Also if $v_r \notin \text{Per}(D_2)$, then since $\text{ecc}(u_i, v_r) < n$, $(u_i, v_r) \notin \text{Per}(D_1 \boxtimes D_2)$. Hence it follows that $\text{Per}(D_1 \boxtimes D_2) = V(D_1) \times \text{Per}(D_2)$.

2. Let $\text{diam}(D_1) = \text{diam}(D_2) = n$. If $u_i \in \text{Per}(D_1)$, then for all $v_r \in V(D_2)$, $(u_i, v_r) \in \text{Per}(D_1 \boxtimes D_2)$, since $\text{ecc}(u_i, v_r) = \max\{\text{ecc}(u_i), \text{ecc}(v_r)\} = n$. Hence $(u_i, v_r) \in \text{Per}(D_1 \boxtimes D_2)$. Similarly, if $v_r \in \text{Per}(D_2)$, then for all $u_i \in V(D_1)$, $(u_i, v_r) \in \text{Per}(D_1 \boxtimes D_2)$. Hence it follows that $[\text{Per}(D_1) \times V(D_2)] \cup [V(D_1) \times \text{Per}(D_2)] \subseteq \text{Per}(D_1 \boxtimes D_2)$.

Conversely, if $(u_i, v_r) \in \text{Per}(D_1 \boxtimes D_2)$, then $\text{ecc}(u_i, v_r) = \max\{\text{diam}(D_1), \text{diam}(D_2)\} = n$. Thus, at least one of $\text{ecc}(u_i)$ and $\text{ecc}(v_r)$ must be necessarily equal to n . Hence $u_i \in \text{Per}(D_1)$ or $v_r \in \text{Per}(D_2)$, and therefore, $\text{Per}(D_1 \boxtimes D_2) \subseteq [\text{Per}(D_1) \times V(D_2)] \cup [V(D_1) \times \text{Per}(D_2)]$. \square

Theorem 3.7. *Let D_1 and D_2 be two strongly connected digraphs.*

1. *If $\text{rad}(D_1) = \text{rad}(D_2)$, then*

$$\text{Ecc}(D_1 \boxtimes D_2) = [\text{Ecc}(D_1) \times V(D_2)] \cup [V(D_1) \times \text{Ecc}(D_2)].$$

2. *If $\text{rad}(D_1) < \text{rad}(D_2)$, then*

$$\text{Ecc}(D_1 \boxtimes D_2) = \left[\bigcup_{\text{ecc}(u_i) \geq \text{rad}(D_2)} \text{Ecc}(u_i) \times V(D_2) \right] \cup [V(D_1) \times \text{Ecc}(D_2)].$$

Proof.

1. First we will prove that $\text{Ecc}(D_1 \boxtimes D_2) \subseteq [\text{Ecc}(D_1) \times V(D_2)] \cup [V(D_1) \times \text{Ecc}(D_2)]$. Let $(u_i, v_r) \in \text{Ecc}(D_1 \boxtimes D_2)$. Then there exists a vertex (u_j, v_s) such that $\text{ecc}(u_j, v_s) = d((u_j, v_s), (u_i, v_r)) = \max\{d(u_j, u_i), d(v_s, v_r)\}$. Since $\text{ecc}(u_j, v_s) = \max\{\text{ecc}(u_j), \text{ecc}(v_s)\}$, and $\text{ecc}(u_j) \geq d(u_j, u_i)$ and $\text{ecc}(v_s) \geq d(v_s, v_r)$, at least one of $\text{ecc}(u_j) = d(u_j, u_i)$ and $\text{ecc}(v_s) = d(v_s, v_r)$ must hold. So necessarily u_i is an eccentric vertex of u_j , or v_r is an eccentric vertex of v_s .

Hence $(u_i, v_r) \in [\text{Ecc}(D_1) \times V(D_2)] \cup [V(D_1) \times \text{Ecc}(D_2)]$.

Let $\text{rad}(D_1) = \text{rad}(D_2) = n$. Let $u_i \in \text{Ecc}(D_1)$. Then there exists a vertex $u_j \in V(D_1)$ such that $\text{ecc}(u_j) = d(u_j, u_i)$. Consider the vertex $(u_i, v_r) \in V(D_1 \boxtimes D_2)$, where v_r is an arbitrary vertex in D_2 . Since $\text{rad}(D_2) = n$, there exists a vertex $v_s \in V(D_2)$ such that $\text{ecc}(v_s) = n$. Hence $d(v_s, v_r) \leq n$ and so $\text{ecc}(u_j, v_s) = \max\{\text{ecc}(u_j), \text{ecc}(v_s)\} = \max\{\text{ecc}(u_j), n\} = \text{ecc}(u_j)$. Thus, $d((u_j, v_s), (u_i, v_r)) = \max\{d(u_j, u_i), d(v_s, v_r)\} = \text{ecc}(u_j) = \text{ecc}(u_j, v_s)$. So (u_i, v_r) is an eccentric vertex of (u_j, v_s) . Thus if $u_i \in \text{Ecc}(D_1)$, then $(u_i, v_r) \in \text{Ecc}(D_1 \boxtimes D_2)$ for all $v_r \in V(D_2)$. Similarly, we can prove that if $v_q \in \text{Ecc}(D_2)$, then $(u_k, v_q) \in \text{Ecc}(D_1 \boxtimes D_2)$ for all $u_k \in V(D_1)$.

Hence $[\text{Ecc}(D_1) \times V(D_2)] \cup [V(D_1) \times \text{Ecc}(D_2)] \subseteq \text{Ecc}(D_1 \boxtimes D_2)$, and so the result holds.

2. Let $\text{rad}(D_1) < \text{rad}(D_2) = n$. Let $u_i \in V(D_1), v_r \in V(D_2)$. Here two cases arise:

Case 1. $v_r \in \text{Ecc}(D_2)$.

Then there exists a vertex $v_s \in V(D_2)$ such that $\text{ecc}(v_s) = d(v_s, v_r)$. Let $u_p \in V(D_1)$ be such that $\text{ecc}(u_p) = \text{rad}(D_1)$. Then since $\text{rad}(D_2) > \text{ecc}(u_p)$, $\text{ecc}(u_p, v_s) = \max\{\text{ecc}(u_p), \text{ecc}(v_s)\} = \text{ecc}(v_s)$. Also, $d((u_p, v_s), (u_i, v_r)) = \max\{d(u_p, u_i), d(v_s, v_r)\} = \text{ecc}(v_s)$. Thus, (u_i, v_r) is an eccentric vertex of (u_p, v_s) . So in this case, $V(D_1) \times \text{Ecc}(D_2) \subseteq \text{Ecc}(D_1 \boxtimes D_2)$.

Case 2. $v_r \notin \text{Ecc}(D_2)$.

Let $v_q \in V(D_2)$ be such that $\text{ecc}(v_q) = \text{rad}(D_2)$. Let $\bigcup_{\text{ecc}(u_i) \geq \text{rad}(D_2)} \text{Ecc}(u_i) = A$. Let $u_k \in A$. Then there exists a vertex $u_p \in V(D_1)$ such that $\text{ecc}(u_p) \geq \text{rad}(D_2)$ and $\text{ecc}(u_p) = d(u_p, u_k)$. Then $d((u_p, v_q), (u_k, v_r)) = \max\{d(u_p, u_k), d(v_q, v_r)\} = d(u_p, u_k) = \text{ecc}(u_p) = \text{ecc}(u_p, v_q)$ and hence (u_k, v_r) is an eccentric vertex of (u_p, v_q) . Hence in this case, $\bigcup_{\text{ecc}(u_i) \geq \text{rad}(D_2)} \text{Ecc}(u_i) \times V(D_2) \subseteq \text{Ecc}(D_1 \boxtimes D_2)$.

Thus, $[\bigcup_{\text{ecc}(u_i) \geq \text{rad}(D_2)} \text{Ecc}(u_i) \times V(D_2)] \cup [V(D_1) \times \text{Ecc}(D_2)] \subseteq \text{Ecc}(D_1 \boxtimes D_2)$.

Conversely, let $(u_k, v_r) \in \text{Ecc}(D_1 \boxtimes D_2)$. Then there exists a vertex $(u_j, v_s) \in V(D_1 \boxtimes D_2)$ such that $\text{ecc}(u_j, v_s) = d((u_j, v_s), (u_k, v_r)) = \max\{d(u_j, u_k), d(v_s, v_r)\} = \max\{\text{ecc}(u_j), \text{ecc}(v_s)\}$. If $v_r \in \text{Ecc}(D_2)$, we get $(u_k, v_r) \in V(D_1) \times \text{Ecc}(D_2)$.

Hence suppose that $(u_k, v_r) \in \text{Ecc}(D_1 \boxtimes D_2)$ and $v_r \notin \text{Ecc}(D_2)$. Then for all $v_s \in V(D_2)$, $\text{ecc}(v_s) > d(v_s, v_r)$. Thus, $\text{ecc}(u_j, v_s) = \text{ecc}(u_j) = d(u_j, u_k)$. If possible, suppose that $u_k \notin A = \bigcup_{\text{ecc}(u_i) \geq \text{rad}(D_2)} \text{Ecc}(u_i)$. Thus, there is no vertex u_j in D_1 such that $\text{ecc}(u_j) = d(u_j, u_k)$ and $\text{ecc}(u_j) \geq \text{rad}(D_2)$. Hence if u_k is an eccentric vertex of u_j in D_1 , then $d(u_j, u_k) < \text{rad}(D_2)$. We have, $\text{rad}(D_1 \boxtimes D_2) = \max\{\text{rad}(D_1), \text{rad}(D_2)\} = \text{rad}(D_2)$. Thus, (u_k, v_r) cannot be the eccentric vertex of any vertex $(u_j, v_s) \in D_1 \boxtimes D_2$, since $d((u_j, v_s), (u_k, v_r)) = \max\{d(u_j, u_k), d(v_s, v_r)\} \neq \text{ecc}(u_j, v_s)$ in this case. This is a contradiction, and hence $u_k \in A$. Hence $(u_k, v_r) \in \bigcup_{\text{ecc}(u_i) \geq \text{rad}(D_2)} \text{Ecc}(u_i) \times V(D_2)$.

Hence $\text{Ecc}(D_1 \boxtimes D_2) \subseteq [\bigcup_{\text{ecc}(u_i) \geq \text{rad}(D_2)} \text{Ecc}(u_i) \times V(D_2)] \cup [V(D_1) \times \text{Ecc}(D_2)]$. □

Theorem 3.8. Let D_1 and D_2 be two strongly connected digraphs. Then $\text{Ct}(D_1 \boxtimes D_2) = A_1 \cup A_2 \cup A_3$, where

$$A_1 = [\text{Ct}(D_1) \times \text{Ct}(D_2)],$$

$$A_2 = \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \text{Ct}(D_1), v_r \notin \text{Ct}(D_2), \text{ and } \text{ecc}(v_q) \leq \text{ecc}(u_i) \text{ for all } v_q \in N[v_r]\},$$

$$A_3 = \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \notin \text{Ct}(D_1), v_r \in \text{Ct}(D_2), \text{ and } \text{ecc}(u_k) \leq \text{ecc}(v_r) \text{ for all } u_k \in N[u_i]\}.$$

Proof. $(u_i, v_r) \in \text{Ct}(D_1 \boxtimes D_2)$ if and only if $\text{ecc}(u_i, v_r) \geq \text{ecc}(u_k, v_q)$ for all $(u_k, v_q) \in N[(u_i, v_r)]$; if and only if $\max\{\text{ecc}(u_i), \text{ecc}(v_r)\} \geq \max\{\text{ecc}(u_k), \text{ecc}(v_q)\}$ for all $u_k \in N[u_i]$ and $v_q \in N[v_r]$; if and only if one of the following three cases holds.

1. $\max\{\text{ecc}(u_i), \text{ecc}(v_r)\} = \text{ecc}(u_i) = \text{ecc}(v_r)$. Then, $\text{ecc}(u_i) \geq \text{ecc}(u_k)$ and $\text{ecc}(v_r) \geq \text{ecc}(v_q)$ for all $u_k \in N[u_i]$ and $v_q \in N[v_r]$.
2. $\max\{\text{ecc}(u_i), \text{ecc}(v_r)\} = \text{ecc}(u_i) > \text{ecc}(v_r)$. Then, $\text{ecc}(u_i) \geq \text{ecc}(u_k)$ for all $u_k \in N[u_i]$ and $\text{ecc}(v_r) < \text{ecc}(u_i), \text{ecc}(v_q) \leq \text{ecc}(u_i)$ for all $v_q \in N(v_r)$.

3. $\max\{\text{ecc}(u_i), \text{ecc}(v_r)\} = \text{ecc}(v_r) > \text{ecc}(u_i)$. Then, $\text{ecc}(v_r) \geq \text{ecc}(v_q)$ for all $v_q \in N[v_r]$ and $\text{ecc}(u_i) < \text{ecc}(v_r)$, $\text{ecc}(u_k) \leq \text{ecc}(v_r)$ for all $u_k \in N(u_i)$.

In case 1, $(u_i, v_r) \in \text{Ct}(D_1 \boxtimes D_2)$.

In case 2, $(u_i, v_r) \in \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \text{Ct}(D_1), v_r \notin \text{Ct}(D_2), \text{ and } \text{ecc}(v_q) \leq \text{ecc}(u_i) \text{ for all } v_q \in N[v_r]\}$.

In case 3, $(u_i, v_r) \in \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \notin \text{Ct}(D_1), v_r \in \text{Ct}(D_2), \text{ and } \text{ecc}(u_k) \leq \text{ecc}(v_r) \text{ for all } u_k \in N[u_i]\}$.

Thus we get, $\text{Ct}(D_1 \boxtimes D_2) = A_1 \cup A_2 \cup A_3$. □

Consider the contour set of the strong product of two connected undirected graphs. As in the case of the boundary set, the result holds even when the undirected graphs are not simple.

Corollary 3.9. *Let D_1 and D_2 be two connected undirected graphs. Then*

$$\begin{aligned} \text{Ct}(D_1 \boxtimes D_2) &= \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \text{Ct}(D_1), v_r \notin \text{Ct}(D_2), \text{ and} \\ &\hspace{15em} \text{ecc}(v_r) < \text{ecc}(u_i)\} \\ &\cup \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \notin \text{Ct}(D_1), v_r \in \text{Ct}(D_2), \text{ and} \\ &\hspace{15em} \text{ecc}(u_i) < \text{ecc}(v_r)\} \\ &\cup [\text{Ct}(D_1) \times \text{Ct}(D_2)]. \end{aligned}$$

Proof. By Theorem 3.8, when D_1 and D_2 are two strongly connected digraphs, $\text{Ct}(D_1 \boxtimes D_2) = A_1 \cup A_2 \cup A_3$. Since D_1 and D_2 are given to be undirected graphs, eccentricity of two adjacent vertices differ by atmost one. Hence

$$A_1 = \text{Ct}(D_1) \times \text{Ct}(D_2),$$

$$\begin{aligned} A_2 &= \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \text{Ct}(D_1), v_r \notin \text{Ct}(D_2), \text{ and} \\ &\hspace{15em} \text{ecc}(v_q) \leq \text{ecc}(u_i) \text{ for all } v_q \in N[v_r]\} \\ &= \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \text{Ct}(D_1), v_r \notin \text{Ct}(D_2), \text{ and} \\ &\hspace{15em} \text{ecc}(v_r) + 1 \leq \text{ecc}(u_i)\} \\ &= \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \text{Ct}(D_1), v_r \notin \text{Ct}(D_2), \text{ and } \text{ecc}(v_r) < \text{ecc}(u_i)\}, \end{aligned}$$

$$A_3 = \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \notin \text{Ct}(D_1), v_r \in \text{Ct}(D_2), \text{ and } \text{ecc}(u_i) < \text{ecc}(v_r)\},$$

since $\max_{u_k \in N[u_i]} \text{ecc}(u_k) = \text{ecc}(u_i) + 1$. Hence it follows that

$$\begin{aligned} \text{Ct}(D_1 \boxtimes D_2) &= \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \in \text{Ct}(D_1), v_r \notin \text{Ct}(D_2), \text{ and} \\ &\hspace{15em} \text{ecc}(v_r) < \text{ecc}(u_i)\} \\ &\cup \{(u_i, v_r) \in V(D_1 \boxtimes D_2) : u_i \notin \text{Ct}(D_1), v_r \in \text{Ct}(D_2), \text{ and} \\ &\hspace{15em} \text{ecc}(u_i) < \text{ecc}(v_r)\} \\ &\cup [\text{Ct}(D_1) \times \text{Ct}(D_2)]. \end{aligned} \quad \square$$

We have examined the boundary-type sets of the strong product of two strongly connected digraphs D_1 and D_2 . Now suppose that at least one of D_1 and D_2 , say D_1 , is not strongly connected. Then the eccentricity of every vertex in D_1 is infinity, and hence the


eccentricity of every vertex in $D_1 \boxtimes D_2$ is infinity. Thus, we have $\partial(D_1) = \text{Per}(D_1) = \text{Ecc}(D_1) = \text{Ct}(D_1) = V(D_1)$, and $\partial(D_1 \boxtimes D_2) = \text{Per}(D_1 \boxtimes D_2) = \text{Ecc}(D_1 \boxtimes D_2) = \text{Ct}(D_1 \boxtimes D_2) = V(D_1) \times V(D_2)$. Since $\text{rad}(D_1) = \text{diam}(D_1) = \infty$, the expression for $\text{Per}(D_1 \boxtimes D_2)$ in Theorem 3.6, and the expression for $\text{Ecc}(D_1 \boxtimes D_2)$ in Theorem 3.7 gives $V(D_1) \times V(D_2)$. Since $\text{ecc}(u_i) = \infty$ for all $u_i \in V(D_1)$, the expression for $\partial(D_1 \boxtimes D_2)$ in Theorem 3.3, and the expression for $\text{Ct}(D_1 \boxtimes D_2)$ in Theorem 3.8 also gives $V(D_1) \times V(D_2)$. Similar is the case when D_2 and both D_1 and D_2 are not strongly connected.


Thus, the results derived for the boundary-type sets of the strong product of two strongly connected digraphs D_1 and D_2 hold also when the digraphs D_1 and D_2 are not even weakly connected. So the results for the boundary-type sets of the strong product of two connected undirected graphs hold for any two arbitrary undirected graphs.

4 Conclusion


In this article, the relationship between the boundary-type sets of the strong product of two digraphs, and that of its factors is derived. As ‘maximum distance’ is the generalization of the usual distance in an undirected graph, these results hold for undirected graphs also. The results for the periphery and eccentricity sets of the strong product of two undirected graphs turn out to be the same as the results in [4]. The results for the boundary and contour sets in the undirected case, as described in [4], are also derived as special cases.

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