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Upper bounds on scrambling index for non-primitive digraphs

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ABSTRACT

The notion of the scrambling index is a fundamental invariant in graph theory and in the theory of non-negative matrices and their applications. Namely, a scrambling index of a primitive directed graph G is the smallest positive integer $k = k(G)$ such that for any pair of vertices u,v of G there exists a vertex w of G such that there are directed walks of length k from u to w and from v to w. In this paper, we generalize the definition to arbitrary directed graphs. We describe constructively the class of graphs with non-zero scrambling index and generalize the Akelbek–Kirkland bounds for the scrambling index to arbitrary directed graphs. Also, the directed graphs with extremal scrambling index are characterized.

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1. Introduction

1.1. Directed graphs

Terminology and notation used here follow [1]. Let $G = (V, E)$ denote a directed graph (digraph). Let $V = V(G)$, $E = E(G)$ and $n = |G| = |V|$ be its vertex set, its edge set and its order, correspondingly. Loops are permitted but multiple edges are not. A digraph H is called a subgraph of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G) \cap (V(H) \times V(H))$. A directed walk from u to v in G is a sequence of vertices $u, w_1, \dots, w_l, v \in V(G)$ and a sequence of edges $(u, w_1), (w_1, w_2), \dots, (w_l, v) \in E(G)$, where vertices and edges are not necessarily distinct. A walk without repeating vertices is called simple. The length of a walk is the number of edges in it. The notation $u \xrightarrow{l} v$ is used to indicate that there is a directed walk of length l from u to v, where $u, v \in V(G)$. If there exists a directed walk from u to v, then the distance between u and v is the number $d(u, v) = \min\{l \geqslant 0 \mid u \xrightarrow{l} v\}$. Otherwise, we say that $d(u, v) = \infty$. For a positive integer m, G^m denotes the digraph with the vertex set $V(G)$ and the edge set $E(G^m) = \{(u, v) \mid u \xrightarrow{m} v \text{ in } G\}$.

A directed walk from u to v is called a closed directed walk or a directed cycle if $u = v$. We denote by $\sigma(G)$ the greatest common divisor of lengths of all closed directed walks in G. If there are no such walks, we say $\sigma(G) = \infty$. An elementary cycle is a closed directed

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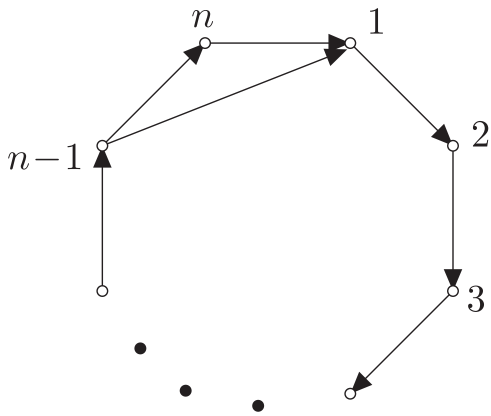


Figure 1. Wielandt's digraph W_n.

walk with no repeating vertices. The girth of G is the minimal length of elementary cycles of G.

Digraphs of order n are naturally related to square non-negative matrices of order n. Indeed, for a square non-negative matrix $A = (a_{ij})$ of order n, its associated digraph is defined to be the digraph $G(A)$ such that $V(G(A)) = \{v_1, \dots, v_n\}$ and $G(A)$ has an edge from v_i to v_j if and only if $a_{ij} \neq 0$. Conversely, the adjacency matrix of a digraph G with $V(G) = \{v_1, \dots, v_n\}$ is the square $(0, 1)$-matrix $A(G)$ of order n such that $A(G)(i, j) = 1$ if and only if there exists an edge from v_i to v_j in G. It is well known that for an arbitrary integer $m > 0$, $A(G^m) = A(G)^m$. Note that this is not a unique possible way to connect these notions, see, for example [2] and references therein.

Digraphs G_1 and G_2 are called isomorphic if there is a bijection $\rho : V(G_1) \to V(G_2)$ such that for each pair $u, v \in V(G_1)$ it holds that $(u, v) \in E(G_1)$ if and only if $(\rho(u), \rho(v)) \in E(G_2)$. An isomorphism of digraphs is denoted by $\cong$, i.e. $G_1 \cong G_2$.

A digraph G is called primitive if there exists a positive integer t such that $u \xrightarrow{t} v$ for arbitrary vertices u,v of G. Note that a digraph consisting of just one vertex with a loop is primitive, however, without this loop it is not. If G is primitive, the smallest such t is called the exponent of G, denoted by $\exp(G)$. It is well known that G is primitive if and only if G is strongly connected and $\sigma(G) = 1$ (see [1, Theorem 3.4.4]).

Example 1.1: A classical example of a primitive digraph is the Wielandt digraph W_n, $n \geqslant 2$, with the vertex set $V = \{1, 2, \dots, n\}$ and the edge set

$$E = \{(1, 2), (2, 3), \dots, (n-1, n), (n, 1)\} \cup \{(n-1, 1)\}$$

(see Figure 1). W_n is primitive, because it has two closed walks of lengths $n-1$ and n, correspondingly.

The following inequality was stated by Wielandt in 1950. It establishes an upper bound on exponents of primitive digraphs of order n (see [1, p. 82]) and will be important for our further considerations.

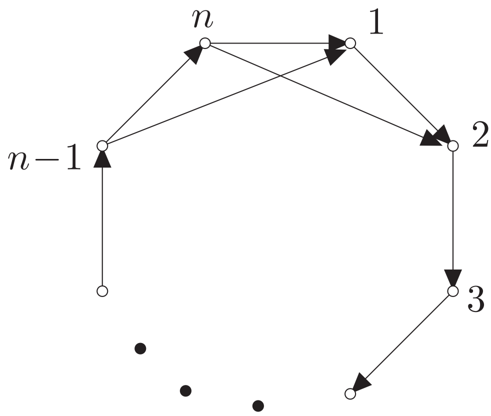


Figure 2. Digraph W'_n.

Theorem 1.2: *Let G be a primitive digraph of order $n \geqslant 2$. Then*

$$\exp(G) \leqslant (n-1)^2 + 1.$$

The equality holds if and only if $G \cong W_n$.

Below we present one more digraph of order n with the girth $n-1$. This digraph will be used later for our classification results.

Example 1.3: Let W'_n be the digraph such that $V(W'_n) = V(W_n)$ and $E(W'_n) = E(W_n) \cup \{(n, 2)\}$ (see Figure 2). It is known that $\exp(W'_n) = (n-1)^2$ (see [1, pp. 82–83]).

1.2. Scrambling index

The notion of the scrambling index is a fundamental invariant in graph theory and in the theory of non-negative matrices and their applications considered by Paz in [3] and by Seneta in [4]. Recently the investigation of the scrambling index and its applications became an active research topic in graph theory, see [5–17]. It is defined for primitive digraphs by Akelbek and Kirkland in [7]. Here we extend this notion without changes to all digraphs.

Definition 1.4: A *scrambling index* of a directed graph G is the smallest positive integer k such that for each pair of vertices $u, v \in V(G)$, there exists a vertex $w \in V(G)$ such that $u \xrightarrow{k} w$, $v \xrightarrow{k} w$. We denote this number by $k(G)$. If there is no such k, we say that $k(G) = 0$.

Remark 1.5: For a primitive digraph G, we have $0 < k(G) \leqslant \exp(G)$ as follows from the definitions of $k(G)$ and $\exp(G)$.

The scrambling index is important with respect to several applications. In particular, let A be an $n \times n$ non-negative primitive stochastic matrix with a non-unit eigenvalue λ.

Let k be the scrambling index of $G(A)$. Then it is proved in [7] that $|\lambda| \leq (\tau_1(A^k))^{1/k} < 1$, where $\tau_1(A^k) = \frac{1}{2}\max_{i,j}\sum_{l=1}^{n}|a_{il}^{(k)} - a_{jl}^{(k)}|$ is the Dobrushin coefficient (also called Δ-coefficient). This coefficient is actively used for the investigations of Markov chains, see [3,4].

Another application lies in the theory of communication (see [14,18]). One may consider a memoryless communication system, which is represented by a digraph G of order n. Suppose that at time $t=0$ each of two different vertices of G (in general, two may be replaced with an arbitrary integer λ such that $2 \leqslant \lambda \leqslant n$, see [14] for the details) 'knows' one bit of information and these bits are distinct. At time $t=1$ each vertex having some information in it passes all the information bits to each of its neighbours (according to the edge direction) and simultaneously it may receive some information from other vertices. After that every vertex forgets the information that passed and has only the received information or nothing. The system continues in this way. For some digraphs (e.g. for primitive digraphs), after certain time there exists a vertex that knows both bits of the information, independently on the initial two vertices.

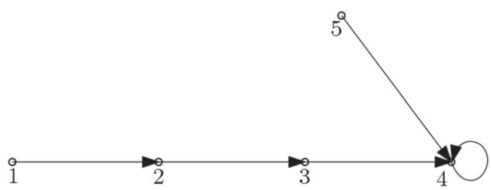
The following two questions arise naturally:

Question 1. For which digraphs such a vertex exists?

Question 2. What is an upper bound for the minimal time necessary for some vertex to know all the information, independently on the initial two vertices?

It is not difficult to verify (see Lemma 2.3) that a digraph G satisfies the condition posed in Question 1 if and only if $k(G) \neq 0$. Moreover, in this case the minimal time from Question 2 equals $k(G)$ (see Corollary 2.4). In particular, for a primitive digraph, there exists a vertex from Question 1 and the upper bounds from Question 2 were stated by Akelbek and Kirkland, see Theorems 1.7 and 1.8. However, the above two problems make sense for all digraphs. There is a large class of non-primitive digraphs satisfying the condition posed in Question 1.

Example 1.6: Consider the following digraph G.



It is not primitive but satisfies the required property. In three steps the vertex 4 knows all the information no matter what the initial vertices were. Thus $k(G) \neq 0$.

The main aim of our paper is to obtain a complete answer to Question 1 and Question 2. Akelbek and Kirkland proved the following upper bounds in the paper [7].

Theorem 1.7: *[7, Theorem 3.17] Let G be a primitive digraph with n vertices and the girth s. Then*

$$k(G) \leqslant K(n, s),$$

where $K(n,s) = n - s + k(n,s)$ and

$$k(n,s) = \begin{cases} \left(\dfrac{s-1}{2}\right) n, & \text{if } s \text{ is odd;} \\ \left(\dfrac{n-1}{2}\right) s, & \text{if } s \text{ is even.} \end{cases}$$

Let $\lceil x \rceil$ denote the smallest integer greater than or equal to x. By J_n, we denote the complete digraph of order n, i.e. the digraph with the vertex set $V(J_n) = \{1, 2, \ldots, n\}$ and the edge set $E(J_n) = \{(i,j) \mid 1 \leqslant i, j \leqslant n\}$.

Theorem 1.8: *[7, Theorem 3.18] Let G be a primitive digraph with $n \geqslant 2$ vertices. Then*

$$k(G) \leqslant \left\lceil \frac{(n-1)^2 + 1}{2} \right\rceil.$$

If $n \geqslant 3$, then the equality holds if and only if $G \cong W_n$. If $n = 2$, then the equality holds if and only if $G \cong W_2$ or $G \cong J_2$.

Remark 1.9: Note that $\lceil ((n-1)^2 + 1)/2 \rceil = K(n, n-1)$.

There are many other bounds on the scrambling index (see, for example [6,7,9,16]), but the most important and general are the bounds from Theorem 1.7 and Theorem 1.8. In view of the above applications, it is useful to know whether or not these bounds remain true for non-primitive digraphs.

To answer all stated questions we first note (see Theorem 3.1) that if G is non-primitive and $k(G) \neq 0$, then G is not strongly connected. This important fact implies that it is sufficient to consider only digraphs that are not strongly connected. Such digraphs have partitions into two subgraphs connected only by edges from one of them to another (see Definition 3.2). In Section 3, for a fixed partition of a digraph, we analyse the connection between the scrambling indices of the subgraph induced by this partition and the whole digraph. Using the concept of graph condensation (see Definition 3.7), we introduce a canonical partition (see Definition 3.10) and develop a technique to estimate the scrambling index of the whole graph. This helps to obtain the results of Sections 4–6.

In Section 4, we characterize the class of digraphs G with $k(G) \neq 0$, answering Question 1. Namely, we prove (see Theorem 4.1) that $k(G) > 0$ if and only if G contains a primitive subgraph satisfying the condition that for any vertex $v \in V(G)$ there exists a directed walk from v to some vertex of this subgraph, see Definition 3.4. Further, we show that the bound given in terms of the girth, see Theorem 1.7, does not hold for non-primitive digraphs. At the same time the general bound, see Theorem 1.8, remains true for all digraphs of the order at least 3 (see Theorem 6.5). Our technique has the following two advantages:

1. It allows to determine constructively if $k(G) = 0$ or not, see Algorithm 4.2.
2. It provides a possibility to generalize Theorems 1.7 and 1.8 to non-primitive digraphs (see Theorems 5.7, 6.1). This means we improve these inequalities for non-primitive

digraphs and characterize the corresponding extremal digraphs. Thus we obtain an answer to Question 2.

Our paper is organized as follows. In Section 2, we compute the numbers $k_{u,v}(G)$ from Definition 2.1 for some important digraphs G. In Section 3, we introduce and investigate some partitions of digraphs, which are a key tool in the further consideration. In Section 4, the digraphs with non-zero scrambling index are characterized and we provide an algorithm to check for a given digraph if its scrambling index is 0 or not. Section 5 is devoted to upper bounds for the scrambling index derived from the partition introduced in Section 3. In Section 6, we obtain general upper bounds and characterize the corresponding extremal digraphs.

2. Some combinatorial indices of the digraphs W_n and W'_n

First we investigate some combinatorial indices that are useful for our further considerations.

Definition 2.1: [7, page 1114] For $u, v \in V(G)$, let

$$k_{u,v}(G) \ = \min\{k \in \mathbb{N} \mid \text{there exists } w \in V(G) \colon u \xrightarrow{k} w, v \xrightarrow{k} w\}.$$

If the set on the right-hand side is empty, then define $k_{u,v}(G) = 0$.

Remark 2.2: Clearly, $k_{u,v}(G) = k_{v,u}(G)$ for each pair $u, v \in V(G)$.

Lemma 2.3: *Let G be an arbitrary digraph. Then $k(G) \neq 0$ if and only if $k_{u,v}(G) \neq 0$ for each pair $u, v \in V(G)$.*

Proof: Let $k(G) = k \neq 0$. Then by Definition 1.4, for two arbitrary vertices u,v of G there exists a vertex w such that $u \xrightarrow{k} w$, $v \xrightarrow{k} w$. Therefore, $k_{u,v}(G) \neq 0$.

Now let us prove the converse. Suppose that $k_{u,v}(G) \neq 0$ for each pair of vertices $u, v \in V(G)$. Define the number

$$k = \max_{u,v \in V(G)} k_{u,v}(G) \neq 0.$$

Let u and v be two arbitrary vertices of G. We are going to prove that there exists a vertex x such that $u \xrightarrow{k} x$ and $v \xrightarrow{k} x$. Since $k_{u,v}(G) \neq 0$, we have that there exists a vertex $w = w_{u,v}$ such that $u \xrightarrow{k_{u,v}(G)} w$, $v \xrightarrow{k_{u,v}(G)} w$. By the condition, it is straightforward to see that each vertex of G has at least one outgoing edge. In particular, w has an outgoing edge ending by w_1. Then w_1 has an outgoing edge ending by w_2, etc. Therefore there exists a vertex $\tilde{w}$ such that $w \xrightarrow{k-k_{u,v}(G)} \tilde{w}$. Hence, $u \xrightarrow{k} \tilde{w}$, $v \xrightarrow{k} \tilde{w}$.

From the arbitrariness of u,v, it follows that $k(G) \neq 0$ and $k(G) \leqslant k$. ■

Corollary 2.4: *Let G be a digraph such that $k(G) \neq 0$. Then*

$$k(G) = \max_{u,\, v \in V(G)} k_{u,v}(G).$$

Proof: By Definition 1.4, $k(G) \geqslant k_{u,v}(G)$ for each pair of vertices u,v of G. Hence, $k(G) \geqslant \max_{u,\,v\in V(G)} k_{u,v}(G)$. Also, it follows directly from the proof of Lemma 2.3 that $k(G) \leqslant \max_{u,\,v\in V(G)} k_{u,v}(G)$. Therefore, $k(G) = \max_{u,\,v\in V(G)} k_{u,v}(G)$ as required. ∎

Next proposition allows one to compute all possible values $k_{u,v}(W_n)$.

Proposition 2.5: *Let $n \geqslant 3$, $n > u > v \geqslant 1$ and $n > t \geqslant 1$. Then*

1. $k_{u,v}(W_n) = \min\{(u-v)n - u + 1, (n+v-u-1)n - v + 1\}$.
2. $k_{n,t}(W_n) = 1 + \min\{t(n-1), (n-t-1)n\}$.

Proof:

1. The digraph W_n contains a unique elementary cycle of length n and a unique elementary cycle of length $n-1$. We denote them by L_n and C_{n-1}, correspondingly.

By Remark 1.5 and Lemma 2.3, $k_{u,v}(W_n) > 0$. Hence by Definition 2.1 there exists a vertex w attainable from u and v by directed walks of the same length. Let us denote such walks of minimal possible lengths by γ_1 and γ_2, correspondingly. So, γ_1 is the walk from u to w, γ_2 is the walk from v to w and $|\gamma_1| = |\gamma_2| = k_{u,v}(W_n)$.

In the sequel, we need the following properties of these walks:

(a) Both walks γ_1 and γ_2 cannot terminate by the same edge; otherwise, this edge can be removed that contradicts length minimality of γ_1 and γ_2.

(b) Similarly to Item (a), if γ_1 contains a cycle, then γ_2 does not contain the same cycle and vice versa.

(c) In fact, the terminate vertex $w = 1$. Indeed, if $w \neq 1$, then both walks γ_1 and γ_2 are terminated by the simple walk from 1 to w, since only 1 has more than one ingoing edge. This contradicts Item (a).

(d) It is impossible that both walks γ_1 and γ_2 contain the edge $(n,1)$. Indeed, if $(n,1)$ belongs to γ_1 and γ_2, then also $(n-1,n)$ belongs to both γ_1 and γ_2, since the vertex n has only one ingoing edge. Hence one may replace the walk $(n-1) \to n \to 1$ with the directed edge $(n-1) \to 1$, making γ_1 and γ_2 shorter by 1. This contradicts length minimality of γ_1 and γ_2.

(e) However, the edge $(n,1)$ belongs to γ_1 or γ_2 (and therefore it belongs to exactly one of γ_1 and γ_2). Otherwise, by Item (d), both walks terminate by the edge $(n-1,1)$, contradicting Item (a).

It follows from Items (a), (c), (e) that either γ_1 terminates by the edge $(n,1)$ and γ_2 terminates by the edge $(n-1,1)$ or vice versa. Consider these two cases separately:

Case 1. The walk γ_1 terminates by $(n,1)$ and the walk γ_2 terminates by $(n-1,1)$. Then by Item (d) the edge $(n,1)$ does not belong to γ_2. It follows that γ_2 consists of the simple walk from v to 1 through the edge $(n-1,1)$ (of length $n-v$) and, possibly, several cycles C_{n-1}. We say that γ_2 contains l cycles C_{n-1}, where $l \geqslant 0$. Therefore,

$$|\gamma_2| = l(n-1) + n - v. \tag{1}$$

Surely, $v \xrightarrow{l'(n-1)+n-v} 1$ for an arbitrary $l' \geqslant 0$.

Furthermore, the edge $(n-1,1)$ does not belong to γ_1. Indeed, otherwise, γ_1 contains C_{n-1}, since γ_1 contains the edges $(n-1,1)$ and $(n,1)$. By Item (b), γ_1 and γ_2 cannot both contain C_{n-1}. So, the only possibility for $(n-1,1)$ to belong to γ_1 is that $l=0$. However, in this case by (1) we have that $|\gamma_2| \leqslant n-1 < n \leqslant |\gamma_1|$, since γ_1 contains C_{n-1} (of length $n-1$) and $(n,1)$. This contradiction concludes that γ_1 does not contain $(n-1,1)$, therefore γ_1 goes from u to 1 (by $n-u+1$ steps) and then goes through L_n for some m times, where $m \geqslant 0$. Hence,

$$|\gamma_1| = mn + n - u + 1. \tag{2}$$

Moreover, $u \overset{m'n+n-u+1}{\longrightarrow} 1$ for an arbitrary $m' \geqslant 0$.

Combining (1) and (2), we obtain the Diophantine equation:

$$l(n-1) - v = mn - u + 1. \tag{3}$$

It follows from (3) that

$$l = u - v - 1 + (l-m)n,$$

i.e. $l \equiv u - v - 1 \pmod{n}$. The direct substitution shows that $m = l = u - v - 1$ is a solution of (3). Since $0 \leqslant u - v - 1 < n$, it is the minimal nonnegative solution. Substituting these values to (2) and (1) and combining similar summands, we obtain

$$k_{u,v}(W_n) = (u-v)n - u + 1.$$

Case 2. The walk γ_1 terminates by $(n-1,1)$ and the walk γ_2 terminates by $(n,1)$. In this case, the roles of u and v are interchanged, thus we have the Diophantine equation:

$$l(n-1) - u = mn - v + 1, \tag{4}$$

where γ_1 goes l times through C_{n-1} and γ_2 goes m times through L_n; $l, m \geqslant 0$. The minimal nonnegative solution of (4) is $m = n + v - u - 2$, $l = n + v - u - 1$, since $l \equiv v - u - 1 \pmod{n}$ and $v < u$. Thus

$$k_{u,v}(W_n) = (n + v - u - 1)n - v + 1.$$

2. From the structure of W_n, it is straightforward to see that if $t < n-1$, then n and t have only one outgoing edge. Therefore, $k_{n,t}(W_n) = 1 + k_{t+1,1}(W_n)$. Using Item 1 with $u = t+1, v = 1$, we obtain that $k_{t+1,1}(W_n) = \min\{t(n-1), (n-t-1)n\}$.

Thus

$$k_{n,t}(W_n) = 1 + k_{t+1,1}(W_n) = 1 + \min\{t(n-1), (n-t-1)n\}.$$

Obviously, for $t = n-1$, we have $k_{n,n-1}(W_n) = 1$. ∎

Using Lemma 2.5, we can get some information about vertex pairs u,v such that $k_{u,v}(W_n)$ close to $k(W_n)$.

Let $k(W_n) = \omega_n = \lceil ((n-1)^2 + 1)/2 \rceil$ (see Theorem 1.8).

Proposition 2.6: *The following properties of W_n $(n \geqslant 3)$ hold:*

1. $k_{n,\lfloor n/2\rfloor}(W_n) = \omega_n$. *If* u,v *are vertices and* $\{u, v\} \neq \{n, \lfloor n/2\rfloor\}$, *then the strict inequality* $k_{u,v}(W_n) < \omega_n$ *holds.*
2. $k_{\lfloor n/2\rfloor+1,1}(W_n) = \omega_n - 1$. *Let* $n \neq 4$, u,v *be vertices,* $\{u, v\} \neq \{\lfloor n/2\rfloor + 1, 1\}$, *and* $\{u, v\} \neq \{n, \lfloor n/2\rfloor\}$. *Then the strict inequality* $k_{u,v}(W_n) < \omega_n - 1$ *holds.*

Proof: The first item was proved in [7, Corollary 3.11], see also [6, Proposition 1.3]. We need only to prove the second item.

Without loss of generality, we may assume that $u > v$. Note that $u \geqslant 2$ in this case. At first we consider the case $u \neq n$. Denote $d = u - v > 0$. By Proposition 2.5, we have

$$k_{u,v}(W_n) = \min\{dn - u + 1, (n - d - 1)n - v + 1\}. \tag{5}$$

Consider the cases of even and odd n separately:

Case 1. n is even. Then $\lceil((n - 1)^2 + 1)/2\rceil - 1 = \omega_n - 1 = (n^2 - 2n)/2$. This case splits into the following three subcases.

Subcase 1.1. $d \leqslant (n - 2)/2$. Since $u \geqslant 2$, then using (5), we obtain

$$k_{u,v}(W_n) \leqslant dn - u + 1 \leqslant \frac{n-2}{2}n - u + 1 \leqslant \frac{n^2 - 2n}{2} - 1$$

with the equalities only if $u = 2$, $d = (n - 2)/2$. Note that in the latter case, we obtain that $v = 1$, $d = u - v = 1$, and therefore $n = 4$. If $n \neq 4$, then we have

$$k_{u,v}(W_n) < \frac{n^2 - 2n}{2} - 1 = \omega_n - 2 < \omega_n - 1. \tag{6}$$

Subcase 1.2. $d = n/2$. Then $dn - u + 1 > (n - d - 1)n - v + 1$, therefore by (5), we get

$$k_{u,v}(W_n) = \left(\frac{n}{2} - 1\right) n - v + 1 \leqslant \frac{n^2 - 2n}{2} = \omega_n - 1$$

with the equality if and only if $v = 1, u = n/2 + 1 = \lfloor n/2\rfloor + 1$.

Subcase 1.3. $d \geqslant (n + 2)/2$. Then by (5)

$$\begin{aligned} k_{u,v}(W_n) &\leqslant (n - d - 1)n - v + 1 \leqslant ((n - 4)/2)n - v + 1 \\ &\leqslant (n^2 - 4n)/2 < (n^2 - 2n - 2)/2 = \omega_n - 2 < \omega_n - 1. \end{aligned} \tag{7}$$

Case 2. n is odd. Then $\omega_n - 1 = (n^2 - 2n + 1)/2$. General situation splits into the following subcases:

Subcase 2.1. $d \neq (n - 1)/2$. Then $d \leqslant (n - 3)/2$ or $n - d - 1 \leqslant (n - 3)/2$. Nevertheless, using (5), one obtains

$$k_{u,v}(W_n) \leqslant \frac{n-3}{2}n - v + 1 \leqslant \frac{n^2 - 3n}{2} < \frac{n^2 - 2n - 1}{2} = \omega_n - 2 < \omega_n - 1. \tag{8}$$

Subcase 2.2. $d = (n - 1)/2$. Then $u \geqslant (n + 1)/2$, $d = n - d - 1$, and by (5) one obtains

$$k_{u,v}(W_n) = \frac{n-1}{2}n - u + 1 \leqslant \frac{n-1}{2}n - \frac{n+1}{2} + 1 = \frac{n^2 - 2n + 1}{2} = \omega_n - 1,$$

moreover, the equality holds if and only if $u = (n + 1)/2 = \lfloor n/2\rfloor + 1$ and $v = 1$.

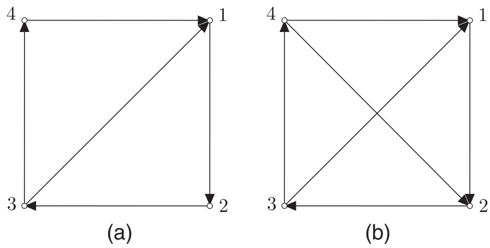


Figure 3. (a) Digraph W_4. (b) Digraph W'_4.

It remains to consider the case $u = n$. We may assume that $v \notin \{\lfloor \frac{n}{2} \rfloor, n-1\}$. From the structure of W_n, it is clear that $k_{n,v}(W_n) = 1 + k_{v+1,1}(W_n) < \omega_n - 1$ by (6)–(8), since $d = (v+1) - 1 = v \neq \lfloor n/2 \rfloor$ by above.

Obviously, $k_{n,n-1}(W_n) = 1 < \omega_n - 1$.

Therefore we proved the required bound in each case, this concludes the proof. ■

Remark 2.7: Assume that $n = 4$. Then $\omega_n = \omega_4 = 5$ and one can directly check (see Figure 3) that

$$k_{1,2}(W_4) = 3, \quad k_{2,3}(W_4) = 2, \quad k_{3,4}(W_4) = 1, \quad k_{4,1}(W_4) = k_{3,1}(W_4) = 4,$$
$$k_{2,4}(W_4) = 5.$$

Hence in the case $n = 4$ Item 2 of Proposition 2.6 does not hold for the pair $\{4, 1\} \neq \{\lfloor n/2 \rfloor + 1, 1\}, \{n, \lfloor n/2 \rfloor\}$.

We also need a similar proposition for the digraph W'_n:

Proposition 2.8: *The following properties of W'_n ($n \geqslant 3$) hold:*

1. *If $u, v \neq n$, then $k_{u,v}(W'_n) = k_{u,v}(W_n)$, in particular, $k_{1,\lfloor n/2 \rfloor + 1}(W'_n) = \omega_n - 1$.*
2. *For each pair of vertices u and v of W'_n such that $\{u, v\} \neq \{1, \lfloor n/2 \rfloor + 1\}$, strict inequality $k_{u,v}(W'_n) < \omega_n - 1$ holds.*
3. *$k(W'_n) = \omega_n - 1$.*

Proof: 1. First we note that W'_n contains two subgraphs isomorphic to W_n. These are $W_n = W'_n - \{(n, 2)\}$ and $W^+_n = W'_n - \{(n-1, 1)\}$. Hence it always holds that $k_{u,v}(W'_n) \leqslant k_{u,v}(W_n)$. Let us consider two directed walks γ_1 and γ_2 with minimal possible length such that there exists a vertex w being attainable from u and v through γ_1 and γ_2, correspondingly. So, $|\gamma_1| = |\gamma_2| = k_{u,v}(W'_n)$.

If both γ_1 and γ_2 do not contain the edge $(n, 2)$, then obviously $k_{u,v}(W'_n) = k_{u,v}(W_n)$. To prove that this is always the case, let us assume without loss of generality that γ_1 contains the edge $(n, 2)$. This edge cannot be the first edge in γ_1, since $u \neq n$. Therefore γ_1 has the previous edge $(n-1, n)$ and one may replace the directed walk $(n-1) \to n \to 2$ with the directed walk $(n-1) \to 1 \to 2$ of the same length. Continuing in the same way, we get that γ_1 and γ_2 both do not contain the edge $(n, 2)$, and the result is proved by above.

2. Let $u > v$. Consider two possible cases:

Case 1. $n = 4$. In this case, $\omega_n = \omega_4 = 5, \{1, \lfloor n/2 \rfloor + 1\} = \{1, 3\}$. One can directly check (see Figure 3) that

$$k_{1,2}(W'_4) = 3, \quad k_{2,3}(W'_4) = 2, \quad k_{3,4}(W'_4) = k_{4,1}(W'_4) = 1, \quad k_{2,4}(W'_4) = 3.$$

All these values are strictly less than $\omega_4 - 1 = 4$ as required.

Case 2. $n \neq 4$. As follows from Proposition 2.6, $k_{u,v}(W'_n) \leqslant k_{u,v}(W_n) < \omega_n - 1$ except for the pairs $(n, \lfloor n/2 \rfloor), (\lfloor n/2 \rfloor + 1, 1)$. But considering the digraph W_n^+ isomorphic to W_n, by Proposition 2.6, Item 2, it follows that

$$k_{n,\lfloor n/2 \rfloor}(W'_n) \leqslant k_{n,\lfloor n/2 \rfloor}(W_n^+) = k_{n-1,\lfloor n/2 \rfloor - 1}(W_n) < \omega_n - 1.$$

3. Follows from two previous items. ■

3. Properties of the scrambling index

The following criterion of primitivity is known and we need it in the sequel. We include here its short proof for the completeness.

Theorem 3.1: *[5, Theorem 3.2.1] Digraph G is primitive if and only if G is strongly connected and $k(G) \neq 0$.*

Proof: Necessity is obvious. Let us prove the sufficient condition.

Let G be strongly connected and $k(G) = k \neq 0$. Then consider an arbitrary edge $(u, v) \in E(G)$. By the definition of the scrambling index there exists a vertex w such that $u \xrightarrow{k} w, v \xrightarrow{k} w$. Hence, $u \xrightarrow{k} w, u \xrightarrow{k+1} w$. Then consider an arbitrary directed walk from w to u of length t. Combining the walks, we find that $u \xrightarrow{k+t} u, u \xrightarrow{k+1+t} u$. This means that G has two closed walks of lengths $k + t$ and $k + t + 1$, which are relatively prime. Therefore we obtain that G is primitive, since G is strongly connected and $\sigma(G) = 1$. ■

Definition 3.2: Let G_1, G_2, G be arbitrary directed graphs. We say that G has a $(G_1 \to G_2)$-partition if G_1 and G_2 are non-empty subgraphs of the digraph G and the following conditions hold:

(i) $V(G_1) \sqcup V(G_2) = V(G)$, i.e. the vertex sets of G_1 and G_2 are disjoint and provide a partition of $V(G)$;
(ii) for each directed edge $e = (v_1, v_2) \in E(G)$, either $e \in E(G_1)$ or $e \in E(G_2)$, or $v_1 \in V(G_1), v_2 \in V(G_2)$.

Remark 3.3: From the geometrical point of view, this means that $V(G)$ is partitioned into two non-intersecting components ($V(G_1)$ and $V(G_2)$) that are connected only by edges from G_1 to G_2.

Definition 3.4: Let G be a digraph, $A \subseteq V(G)$ be a subset. We say that A is *reachable* in G if for any vertex $v \in V(G)$ there exists an $a \in A$ and a number $l \geqslant 0$ such that $v \xrightarrow{l} a$. We say that a subgraph H of G is *reachable* if its vertex set is a reachable set.

For a reachable subgraph H of G and a vertex $u \in V(G)$, we define the distance $d(u, H) = \min_{v \in V(H)} d(u, v)$.

Lemma 3.5: *Let a digraph G have a $(G_1 \to G_2)$-partition. Assume that $k(G) \neq 0$. Then*

1. $k(G_2) \neq 0$ *and* $k(G) \geqslant k(G_2)$,
2. *the subgraph G_2 of G is reachable,*
3. $k_{u,v}(G) \leqslant \max\{d(u, G_2), d(v, G_2)\} + k(G_2)$ for each pair $u, v \in V(G)$,
4. $k(G) \leqslant \max_{u \in V(G_1)} d(u, G_2) + k(G_2) \leqslant |G_1| + k(G_2)$, *where $|G_1|$ is order of the digraph G_1.*

Proof:

1. Let us consider two arbitrary vertices $u, v \in V(G_2)$. Notice that from the definition of $(G_1 \to G_2)$-partition it follows that $k_{u,v}(G_2) = k_{u,v}(G)$ (all the edges of G outgoing from vertices of G_2 are the edges in G_2, so they belong to $E(G_2)$). Consequently, from Lemma 2.3, we have $k(G_2) \neq 0$. Also, by Corollary 2.4, we have $k(G) \geqslant k(G_2)$.
2. Let us consider arbitrary vertices $a \in V(G)$, $b \in V(G_2)$. Then $k_{a,b}(G) \neq 0$, i.e. there exists $a' \in V(G)$ such that $a \xrightarrow{l} a', b \xrightarrow{l} a'$ for some $l \geqslant 0$. It is clear that $a' \in V(G_2)$, since starting at b we can reach only vertices of G_2. We obtain a directed walk from a to $a' \in V(G_2)$, thus G_2 is reachable.
3. Let u and v be two arbitrary vertices of G. By Item 2 there exist vertices $\tilde{u}, \tilde{v} \in V(G_2)$ such that $u \xrightarrow{d(u,G_2)} \tilde{u}, v \xrightarrow{d(v,G_2)} \tilde{v}$. Without loss of generality (up to the exchange of u and v), assume that $d(u, G_2) \geqslant d(v, G_2)$.

Since $k(G) \neq 0$, each vertex of G has at least one outgoing edge. Hence let us consider a vertex $w \in V(G_2)$ such that $\tilde{v} \xrightarrow{d(u,G_2)-d(v,G_2)} w$. One can obtain that $v \xrightarrow{d(u,G_2)} w$ (since $v \xrightarrow{d(v,G_2)} \tilde{v} \xrightarrow{d(u,G_2)-d(v,G_2)} w$). Hence,

$$k_{u,v}(G) \leqslant d(u, G_2) + k_{\tilde{u},w}(G) = d(u, G_2) + k_{\tilde{u},w}(G_2) \leqslant d(u, G_2) + k(G_2).$$

Therefore,

$$k_{u,v}(G) \leqslant \max\{d(u, G_2), d(v, G_2)\} + k(G_2).$$

4. Since u and v are arbitrary, by Corollary 2.4 it follows that

$$k(G) \leqslant \max_{u \in V(G_1)} d(u, G_2) + k(G_2) \leqslant |G_1| + k(G_2),$$

since $d(u, G_2) \leqslant |G_1|$ for an arbitrary vertex u. ■

From Lemma 3.5, we directly obtain the following:

Corollary 3.6: *Let a digraph G has a $(G_1 \to G_2)$-partition. Assume that*

$$k(G) \neq 0 \quad \text{and} \quad k(G) = |G_1| + k(G_2).$$

Then there exists a unique vertex $u \in V(G_1)$ such that $d(u, G_2) = |G_1|$.

Proof: According to Lemma 3.5, Item 4, we have that

$$k(G) = \max_{v \in V(G_1)} d(v, G_2) + k(G_2) = |G_1| + k(G_2),$$

therefore, $\max_{v \in V(G_1)} d(v, G_2) = |G_1|$. Hence there exists $u \in V(G_1)$ such that $d(u, G_2) = |G_1|$. This means that there exists a directed walk of length $|G_1|$ starting with u, ending with some vertex from $V(G_2)$, and containing all the vertices of G_1. Thus for each $\tilde{u} \neq u$, we have $d(\tilde{u}, G_2) < |G_1|$. ■

Recall that two vertices u and v in $V(G)$ are called strongly connected provided there exist directed walks from u to v and from v to u. By the definition, any vertex is strongly connected to itself. Strong connectivity defines an equivalence relation on the vertices of G and yields a partition of $V(G)$ into subsets $V_1, \dots, V_s$.

Definition 3.7: The *condensation* of a digraph G is the digraph $G^\star$ defined in the following way:

1. $V(G^\star) = \{V_1, \dots, V_s\}$, where $V_1, \dots, V_s$ form the discussed above partition of $V(G)$;
2. $(V_i, V_j) \in E(G^\star)$ if and only if $i \neq j$ and there exist $v_i \in V_i$, $v_j \in V_j$ such that $(v_i, v_j) \in E(G)$.

Note that $G^\star$ has no loops. Also, for a strongly connected G, its condensation has only one vertex. Basic properties of $G^\star$ are collected in the following proposition.

Proposition 3.8: *Let G be a digraph, then*

1. *$G^\star$ has no directed cycles.*
2. *$G^\star$ has at least one vertex with no edges outgoing from it.*
3. *The set of all vertices of $G^\star$ with no outgoing edges is reachable.*
4. *If $k(G) \neq 0$, then $G^\star$ has a unique vertex with no edges outgoing from it.*

Proof:
1. Assume that $G^\star$ has a directed cycle. Then all vertices of G belonging to distinct vertices of this directed cycle are equivalent. This contradicts the definition of the condensation.
2. Follows from 1. Indeed, if at least one edge goes from each vertex of $G^\star$, then $G^\star$ has a directed cycle, contrary to 1.
3. Starting at an arbitrary vertex of $G^\star$ we can go out and keep going in an arbitrary way. $G^\star$ has no directed cycles, so finally we end up in a vertex with no outgoing edges.
4. By 2, there exists at least one vertex with no outgoing edges. If we have two (or more) such vertices, V_i and V_j, then consider arbitrary $u \in V_i, v \in V_j$. From the definition of the condensation, it follows that $k_{u,v}(G) = 0$, which contradicts to Lemma 2.3.

■

Consider a digraph G and assume that G is not strongly connected. Its condensation $G^\star$ has the vertices $V_1, \dots, V_s$, $s \geqslant 2$. By Proposition 3.8, it follows that there exists a vertex with no outgoing edges at $G^\star$. Without loss of generality, we can assume that it is V_s.

Let us define digraphs G_1 and G_2 in the following way:

$$V(G_1) = V_1 \cup \cdots \cup V_{s-1},\ E(G_1) = \{(u,v) \mid u,v \in V(G_1), (u,v) \in E(G)\};$$
$$V(G_2) = V_s,\ E(G_2) = \{(u,v) \mid u,v \in V(G_2), (u,v) \in E(G)\}.$$

Corollary 3.9: *If G is a not strongly connected digraph, then G has a $(G_1 \to G_2)$-partition with $V(G_2) \in V(G^\star)$.*

Proof: Whereas V_s in the condensation digraph $G^\star$ has no outgoing edges, we obtain that G has a $(G_1 \to G_2)$-partition. ■

If, in addition, we demand the condition $k(G) \neq 0$, then the vertex in $G^\star$ with no outgoing edges is unique. Let it be the vertex V_s again.

Definition 3.10: In the case $k(G) \neq 0$, we call the described above $(G_1 \to G_2)$-partition of the digraph G the *canonical* partition.

Corollary 3.11: *Let G be a not strongly connected digraph. Assume that $k(G) \neq 0$. Then*

1. *G has the canonical $(G_1 \to G_2)$-partition.*
2. *For the canonical $(G_1 \to G_2)$-partition of G, G_2 is primitive and reachable.*

Proof:

1. Follows by Corollary 3.9.
2. G_2 is strongly connected by Definition 3.10. By Item 1 of Lemma 3.5 it holds that $k(G_2) \neq 0$. Therefore G_2 is primitive by Theorem 3.1. Moreover, the set $\{V(G_2)\}$ is reachable in $G^\star$ (by Proposition 3.8), hence G_2 is reachable in G.

■

The following proposition can be considered as a small improvement of Lemma 3.5 in the simplest case $|G_2| = 1$. We present its proof here for the completeness.

Proposition 3.12: *[12, Proposition 3.5] Let G be a directed graph of order n with a loop at some vertex w. Assume that $k(G) \neq 0$ and there are no outgoing edges from w except this loop. Then $k(G) \leqslant n-1$.*

Proof: We consider an arbitrary vertex a of G. Since $k(G) \neq 0$, by the definition of the scrambling index, we obtain that for an arbitrary vertex a and the vertex w there exists a vertex u such that $a \xrightarrow{k(G)} u$ and $w \xrightarrow{k(G)} u$. Since the only outgoing edge for w is the loop, it follows that $u = w$. Thus there is a walk from a to w for any vertex a. Since G is of order n, there exists a walk from a to w such that $l \leqslant n-1$. Using the loop in w, we get $a \xrightarrow{n-1} w$. Since a is arbitrary, this implies $k(G) \leqslant n-1$. ■

4. Characterization of digraphs with non-zero scrambling index

In this section, we characterize digraphs with non-zero scrambling index and provide an algorithm to check this.

Theorem 4.1: *For an arbitrary digraph G, the following conditions are equivalent:*

1. $k(G) \neq 0$.
2. *There exists a primitive reachable subgraph H of G.*

Proof:

$\underline{1 \Rightarrow 2}$. Let $k(G) \neq 0$. If G is strongly connected, then G is primitive due to Theorem 3.1, so $H = G$. If G is not strongly connected, then consider its canonical $(G_1 \to G_2)$-partition. It now follows that G_2 is a required subgraph by Corollary 3.11.

$\underline{2 \Rightarrow 1}$. Let G have a primitive reachable subgraph H. Consider two arbitrary vertices $u, v \in V(G)$. It follows from the conditions that there exists $w \in V(H)$ such that $u \xrightarrow{l_u} w$, $v \xrightarrow{l_v} w$ for some $l_u, l_v \geqslant 0$. But then from the primitivity of H, one obtains that $w \overset{\exp(H)+l_v}{\longrightarrow} w$ and $w \overset{\exp(H)+l_u}{\longrightarrow} w$. Therefore,

$$u \overset{l_u+\exp(H)+l_v}{\longrightarrow} w, \; v \overset{l_v+\exp(H)+l_u}{\longrightarrow} w.$$

Consequently, $k_{u,v}(G) \neq 0$. Therefore by Lemma 2.3, $k(G) \neq 0$. ∎

We can also notice that for an arbitrary digraph G, the problem to check whether $k(G) = 0$ or not is algorithmically solvable. More precisely, such problem, as can be seen from the algorithm below, reduces to the problem of primitivity test for some strongly connected component of G. Indeed, consider the following algorithm.

Algorithm 4.2:
1. One can find all strongly connected components of G in $O(|V(G)| + |E(G)|)$ time using the classical algorithm of Tarjan (see [19]). These are vertices of condensation $G^\star$.
2. Then we can directly find all the components with no outgoing edges to other components (in linear time). If there are two or more such components, then $k(G) = 0$.
3. Otherwise, there is a unique such component H. Now we need to check whether or not H is primitive. If so, then $k(G) \neq 0$. If not, then $k(G) = 0$.

Remark 4.3: Note that Algorithm 4.2 works in polynomial time, since a primitivity test of a digraph can be done in polynomial time. Indeed, let G be a digraph of order n. By Theorem 1.2, G is primitive if and only if $G^{n^2-2n+2} = J_n$. To compute G^{n^2-2n+2} one may raise $A = A(G)$ to the $(n^2 - 2n + 2)$th power (which obviously is of polynomial time) and then consider its associated digraph $G(A^{n^2-2n+2})$.

Proposition 4.4: *Algorithm 4.2 correctly answers to the question whether* $k(G) = 0$ *or not.*

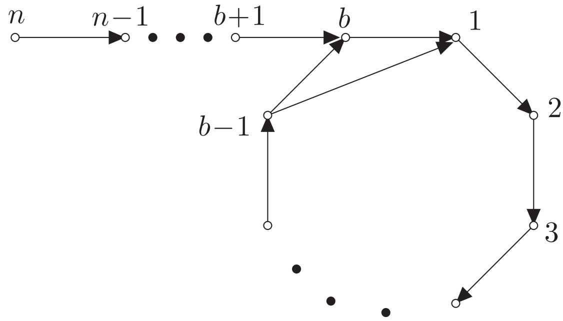


Figure 4. Digraph $H_{n,b}$.

Proof: We first consider Step 2. If there are two or more strongly connected components of G with no outgoing edges to other components, then $k(G) = 0$ by Proposition 3.8, Item 4.

Now proceed to Step 3. Suppose that H is primitive. By Proposition 3.8, Item 3, we have that $\{H\}$ is reachable in $G^\star$, hence H is reachable in G. Therefore Theorem 4.1 states that $k(G) \neq 0$.

Now let us suppose that H is not primitive. Assume that $k(G) \neq 0$. It is obvious that G is not strongly connected, otherwise, $H = G$ is primitive by Theorem 3.1. Then consider the canonical $(G_1 \to G_2)$-partition of G. By Definition 3.10, $G_2 = H$. But from Corollary 3.11, one obtains that H is primitive, a contradiction. Hence, $k(G) = 0$.

Thus the answer of Algorithm 4.2 is correct. ■

5. Upper bounds for the scrambling index derived from the canonical partition

Theorem 5.1: *Let G be a not strongly connected digraph of order n with $k(G) \neq 0$. Consider its canonical $(G_1 \to G_2)$-partition. Let s be the girth of G_2 and $|G_2| = b \leqslant n-1$. Then*

$$k(G) \leqslant n - b + K(b,s).$$

If the equality in the last inequality holds, then $k(G_2) = K(b,s)$ and there exists a unique vertex u of G_1 such that $d(u, G_2) = n - b$.

Proof: By Corollary 3.11, G_2 is primitive. Hence by Theorem 1.7, $k(G_2) \leqslant K(b,s)$. Then we get the required inequality by Lemma 3.5, Item 4. Corollary 3.6 concludes the proof in the equality case. ■

Definition 5.2: For $2 \leqslant b \leqslant n-1$, we define a digraph $H_{n,b}$, see Figure 4, by $V(H_{n,b}) = \{1, 2, \ldots, n\}$ and $E(H_{n,b}) = \{(i, i+1) \mid 1 \leqslant i \leqslant b-1\} \cup \{(b,1),\ (b-1,1)\} \cup \{(j+1, j) \mid b \leqslant j \leqslant n-1\}$:

Lemma 5.3: $k(H_{n,b}) = n - b + \lceil ((b-1)^2 + 1)/2 \rceil$.

Proof: $H_{n,b}$ has a $(G_1 \to G_2)$-partition with $G_2 \cong W_b$ and $|G_1| = n-b$. Hence by Theorem 4.1, $k(H_{n,b}) \neq 0$ and by Lemma 3.5, Item 4,

$$k(H_{n,b}) \leqslant n-b+k(G_2) = n-b+\left\lceil \frac{(b-1)^2+1}{2} \right\rceil.$$

Define the vertex x of $H_{n,b}$ in the following way:

$$x = \begin{cases} \left\lfloor \frac{b}{2} \right\rfloor - (n-b), & \text{if } \left\lfloor \frac{b}{2} \right\rfloor - (n-b) > 0; \\ n - \left\lfloor \frac{b}{2} \right\rfloor, & \text{otherwise.} \end{cases}$$

We note that from the structure of $H_{n,b}$, it follows that any directed walk of length $n-b$ starting at the vertex x has to terminate at the vertex $\lfloor b/2 \rfloor$ (in fact, such a walk is unique). Also, any directed walk of length $n-b$ starting at the vertex n has to terminate at the vertex b (such a walk is unique too).

Now let us calculate $k_{n,x}(H_{n,b})$. From the above, one obtains

$$k_{n,x}(H_{n,b}) = n-b+k_{b,\lfloor b/2 \rfloor}(H_{n,b}) = n-b+k(W_b) = n-b+\lceil ((b-1)^2+1)/2 \rceil,$$

as follows from Proposition 2.6, Item 1. Therefore by Corollary 2.4,

$$k(H_{n,b}) \geqslant k_{n,x}(H_{n,b}) = n-b+\left\lceil \frac{(b-1)^2+1}{2} \right\rceil.$$

■

Theorem 5.4: *Let G be a not strongly connected digraph of order n with $k(G) \neq 0$. Consider its canonical $(G_1 \to G_2)$-partition. Suppose that $|G_2| = b$. Then*

1. $$k(G) \leqslant n-b+\left\lceil \frac{(b-1)^2+1}{2} \right\rceil.$$
2. *If the equality holds, then G contains a subgraph isomorphic to $H_{n,b}$. Furthermore, if vertices of G are labelled as vertices of its subgraph isomorphic to $H_{n,b}$ and G contains an edge $(i,j) \notin E(H_{n,b})$, then $j \geqslant i > b$.*
3. *If the equality holds and $4 \leqslant n < 2b$, then $G \cong H_{n,b}$.*

Proof: 1. If $b=1$, then $k(G) \leqslant n-1 = n-b$ as follows from Proposition 3.12.

Otherwise, $b \geqslant 2$. By Corollary 3.11, G_2 is primitive. Then by Theorem 1.8, $k(G_2) \leqslant \lceil \frac{(b-1)^2+1}{2} \rceil$. Applying Lemma 3.5, Item 4, we obtain

$$k(G) \leqslant n-b+k(G_2) \leqslant n-b+\left\lceil \frac{(b-1)^2+1}{2} \right\rceil.$$

2. Now let us assume that the equality holds. From the above, it follows that $b \geqslant 2$ and $k(G_2) = \lceil ((b-1)^2+1)/2 \rceil$.

Moreover, from Corollary 3.6, there exists a unique vertex $z \in V(G_1)$ such that $d(z, G_2) = n - b$. Consider a vertex $u \in V(G_2)$ with the condition $z \xrightarrow{n-b} u$ by some walk γ (without repeating vertices through this walk). Hence all vertices of G_1 are contained in γ. Suppose they are labelled along this walk in the decreasing order, starting with the vertex $z = n$ (ending with the number $b+1$). Consider two possible cases:

Case 2.1. $b = 2$. Since $|G_2| = b$ and $k(G_2) = \lceil((b-1)^2+1)/2\rceil$, Theorem 1.8 states that $G_2 \cong W_2$ or $G_2 \cong J_2$. Note that the vertex u cannot possess a loop. Otherwise, for each $v \in V(G)$, we have $v \xrightarrow{n-2} u$, therefore, $k(G) \leqslant n-2 < n-1 = n-b+\lceil((b-1)^2+1)/2\rceil$, a contradiction. Hence $G_2 \cong W_2$ and u does not possess a loop. Therefore G obviously contains a subgraph isomorphic to $H_{n,2}$.

Case 2.2. $b \geqslant 3$. Since $|G_2| = b$ and $k(G_2) = \lceil((b-1)^2+1)/2\rceil$, Theorem 1.8 states that $G_2 \cong W_b$. Suppose that G_2 has the same labelling of vertices as in the definition of the Wielandt digraph.

Consider a pair (v, w) of vertices of G such that $v > w$ and $k_{v,w}(G) = k(G) = n - b + \lceil((b-1)^2+1)/2\rceil$. If $v \neq n$, then by Lemma 3.5, Item 3,

$$k_{v,w}(G) \leqslant \max\{d(v, G_2), d(w, G_2)\} + k(G_2) < n - b + k(G_2),$$

this is a contradiction. Therefore, $v = n$ and $n - b + k(W_b) = k(G) = k_{n,w}(G) \leqslant n - b + k_{u,\tilde{w}}(W_b)$, where $\tilde{w}$ is any vertex from $V(G_2)$ such that $w \xrightarrow{n-b} \tilde{w}$. Since $k(W_b) = k_{u,\tilde{w}}(W_b)$, from Proposition 2.6, Item 1, it follows that $u, \tilde{w} \in \{b, \lfloor b/2\rfloor\}, u \neq \tilde{w}$.

We claim that $u = b$. Assume the converse, i.e. $u = \lfloor b/2\rfloor, \tilde{w} = b$. It is sufficient to obtain a contradiction in the case G contains only the edges of $E(G_2)$ and the walk γ. In this case, $z = n \xrightarrow{n-b} \lfloor b/2\rfloor = u, w \xrightarrow{n-b} \tilde{w} \in V(G_2)$. Since $\tilde{w} = b$ has exactly one ingoing edge, we have the walk $w \xrightarrow{n-b-1} (b-1) \xrightarrow{1} 1$ and therefore the walk $w \xrightarrow{n-b} 1$. Note that $1 \notin \{b, \lfloor b/2\rfloor\}$. Hence, $k_{n,w}(G) \leqslant n - b + k_{\lfloor b/2\rfloor,1}(W_b) < k(G)$ by Proposition 2.6, Item 1. A contradiction is obtained. Thus $u = b$ and therefore G contains a subgraph isomorphic to $H_{n,b}$. Moreover, we proved that if $z = n \xrightarrow{n-b} u$, then $u = b$.

Note that in both cases there are no edges of type (i, j) in $E(G)$, where $i > b, i > j$, except for edges of γ, otherwise, $d(z, G_2) = d(n, G_2) < n - b$ (note that if $i = b+1$, then j equals b by the argument above, so (i, j) is an edge of γ). Furthermore, there are no edges of type (i, j) in $E(G)$, where $1 \leqslant i \leqslant b < j$, because of the facts $|G_2| = b$ and G_2 is a strong connectivity component of G. So, the rest edges in $E(G)$ must have type (i, j), where $b < i \leqslant j$. If there are no such edges, then $G \cong H_{n,b}$.

3. Now let $4 \leqslant n < 2b$. Then $b \geqslant 3$. Let us assume that G contains at least one edge (i, j), where $b < i \leqslant j$.

Obviously, this edge and some edges of γ form a cycle C. Since $2b > n$, it follows that $|C| < b$. Denote $|C|$ by l.

Define the vertex x of G in the following way (analogously to Lemma 5.3):

$$x = \begin{cases} \left\lfloor \dfrac{b}{2} \right\rfloor - (n-b), & \text{if } \left\lfloor \dfrac{b}{2} \right\rfloor - (n-b) > 0; \\ n - \left\lfloor \dfrac{b}{2} \right\rfloor, & \text{otherwise.} \end{cases}$$

Recall that if $v > w$ and $k_{v,w}(G) = n - b + \lceil((b-1)^2+1)/2\rceil$, then $v = n$ and for each $\tilde{w} \in V(G_2)$ such that $w \xrightarrow{n-b} \tilde{w}$, it follows that $\tilde{w} = \lfloor b/2 \rfloor$, therefore, $w = x$. Hence (n, x) is the only pair of vertices for which $k(G)$ might be attained. Consider the following cases.

Case 3.1. $l = 1$. In this case, G has a loop at a vertex $y > b$. We have $x \xrightarrow{n-b} \lfloor b/2 \rfloor$, therefore, $x \xrightarrow{n-\lfloor b/2 \rfloor} b$. On the other hand, $n \xrightarrow{n-\lfloor b/2 \rfloor} b$ because of the loop. Thus $k_{n,x}(G) \leqslant n - \lfloor b/2 \rfloor < n - b + \lceil \frac{(b-1)^2+1}{2} \rceil$, while $b \geqslant 3$. A contradiction is obtained.

Case 3.2. $1 < l < \lceil b/2 \rceil$. Starting from the vertex n through the walk γ, then visiting the cycle C once and continuing the walk to the vertex b, one obtains that $n \xrightarrow{n-b+l} b$. On the other hand, $x \xrightarrow{n-b+l} (\lfloor b/2 \rfloor + l)$. Therefore using Proposition 2.5, Item 2, we have

$$\begin{aligned} k_{n,x}(G) &\leqslant n - b + l + k_{b,\lfloor b/2 \rfloor + l}(G) = n - b + l + k_{b,\lfloor b/2 \rfloor + l}(W_b) \\ &\leqslant n - b + l + 1 + \left(b - \left\lfloor \frac{b}{2} \right\rfloor - l - 1\right) b \\ &\leqslant n - b + l + 1 + \left(\frac{b+1}{2} - l - 1\right) b = n - 2b + l + 1 + \frac{b^2+b}{2} - lb. \end{aligned}$$

Since $l < b$, we get

$$k_{n,x}(G) < n - b + 1 + \frac{b^2+b}{2} - lb < n - b + \frac{b^2-2b+2}{2},$$

while $l > \frac{3}{2}$.

Thus $k_{n,x}(G) < n - b + \lceil((b-1)^2+1)/2\rceil$. A contradiction is obtained.

Case 3.3. $l = \lceil b/2 \rceil$. Starting from the vertex n through the walk γ, then visiting the cycle C once and continuing the walk to the vertex b, one obtains that $n \xrightarrow{n-b+l} b$. On the other hand, $x \xrightarrow{n-b+l} (\lfloor b/2 \rfloor + l) = b$. Hence,

$$k_{n,x}(G) \leqslant n - b + l = n - \left\lfloor \frac{b}{2} \right\rfloor < n - b + \left\lceil \frac{(b-1)^2+1}{2} \right\rceil,$$

while $b \geqslant 3$. A contradiction is obtained.

Case 3.4. $b - 1 > l > \lceil b/2 \rceil$. Starting from the vertex n through the walk γ, then visiting the cycle C once and continuing the walk to the vertex b, one obtains that $n \xrightarrow{n-b+l} b$. On the other hand, $x \xrightarrow{n-b+l} (\lfloor b/2 \rfloor + l - b)$. Therefore using Proposition 2.5, Item 2, we have

$$\begin{aligned} k_{n,x}(G) &\leqslant n - b + l + 1 + \left(\left\lfloor \frac{b}{2} \right\rfloor + l - b\right)(b-1) \\ &= n - b + l + 1 + \left(l - \left\lceil \frac{b}{2} \right\rceil\right)(b-1) = n - b + 1 - (b-1)\left\lceil \frac{b}{2} \right\rceil + bl \\ &\leqslant n - b + 1 - \frac{b^2-b}{2} + bl < n - b + \frac{b^2-2b+2}{2}, \end{aligned}$$

while $l < b - \frac{3}{2}$. Consequently, $k_{n,x}(G) < n - b + \lceil ((b-1)^2 + 1)/2 \rceil$. A contradiction is obtained.

Case 3.5. $l = b-1$. Note that in this case $n = 2b-1$, $i = b+1, j = n$. So, $n-b = b-1$.

Denote by L_b the directed cycle $1 \to 2 \to \cdots \to b \to 1$ of G_2.

If b is odd, let us start from the vertex n and visit the cycle C $(b-1)/2$ times, continuing the walk through γ to the vertex b afterwards. As a result we get $n \xrightarrow{n-b+(b-1)\frac{b-1}{2}} b$. At the same time, $x \xrightarrow{\frac{b-1}{2}} b$, through the walk γ. Then visiting the cycle L_b $(b-1)/2$ times, we have $x \xrightarrow{\frac{b-1}{2}+\frac{b-1}{2}b} b$. In fact,

$$n - b + (b-1)\frac{b-1}{2} = \frac{b-1}{2} + \frac{b-1}{2}b = \frac{b^2-1}{2}.$$

Thus $k_{n,x}(G) \leqslant n - b + (b-1)^2/2 < n - b + \lceil ((b-1)^2 + 1)/2 \rceil$. A contradiction is obtained.

Now let b be even. Let us start from the vertex n and visit the cycle C $b/2$ times. So, $x \xrightarrow{(b-1)\frac{b}{2}} x$. Besides $x \xrightarrow{\frac{b}{2}-1} b$ through the walk γ, therefore $x \xrightarrow{(b-1)\frac{b}{2}+\frac{b}{2}-1} b$. At the same time, $n \xrightarrow{b-1} b$, then visiting the cycle L_b $(b/2-1)$ times, we have $n \xrightarrow{b-1+b(\frac{b}{2}-1)} b$. In fact, we obtain the same length. Indeed,

$$(b-1)\frac{b}{2} + \frac{b}{2} - 1 = b - 1 + b\left(\frac{b}{2} - 1\right) = \frac{b^2}{2} - 1.$$

Therefore,

$$k_{n,x}(G) \leqslant \frac{b^2}{2} - 1 < \frac{b^2}{2} = b - 1 + \frac{(b-1)^2+1}{2} = n - b + \left\lceil \frac{(b-1)^2+1}{2} \right\rceil.$$

A contradiction is obtained in this case as well.

Consequently, $G \cong H_{n,b}$. ■

Example 5.5: In the case $n \geqslant 2b$, there exist digraphs satisfying conditions of Theorem 5.4 but non-isomorphic to $H_{n,b}$. For example, let us consider $G = H_{n,b} \cup \{(b+1, 2b)\}$ in the case $n \geqslant 2b$. For $n = 10$, $b = 5$, the corresponding digraph is shown at Figure 5. Evidently, $0 \neq k(G) \leqslant k(H_{n,b})$. Let $x = n - \lfloor b/2 \rfloor$ (analogously to Lemma 5.3). Clearly, by Corollary 2.4 and Theorem 5.4, Item 1, $k_{n,x}(G) \leqslant k(G) \leqslant n - b + \lceil ((b-1)^2 + 1)/2 \rceil$. We are going to show that $k_{n,x}(G) = n - b + \lceil ((b-1)^2 + 1)/2 \rceil$. Then $k(G) = n - b + \lceil ((b-1)^2 + 1)/2 \rceil$.

Let $n = 2b$. Consider the digraph G^b. It is clear that

$$V(G^b) = \{1, \ldots, 2b\},$$
$$E(G^b) = E(W_b) \cup \{(i,i) \mid 1 \leqslant i \leqslant 2b\} \cup \{(i, 2b-i) \mid b+1 \leqslant i < 2b\} \cup \{(2b, b)\}.$$

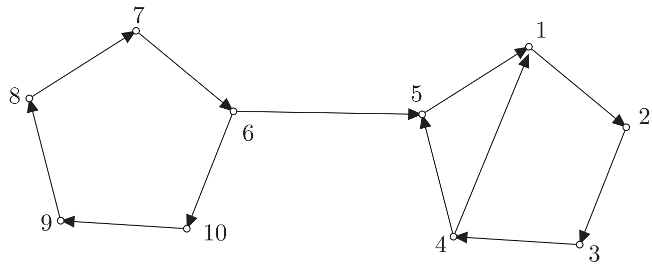


Figure 5. An example of G for $n = 10$, $b = 5$.

Case 1. b is even. Consider vertices $2b$ and x. By the structure of G^b it is easy to see that $k_{2b,x}(G^b) > b/2$. Hence,

$$k_{2b,x}(G) \geqslant \frac{b^2}{2} + 1 = b + \left\lceil \frac{(b-1)^2+1}{2} \right\rceil = n - b + \left\lceil \frac{(b-1)^2+1}{2} \right\rceil.$$

Case 2. b is odd. Note that $n - b + \lceil ((b-1)^2+1)/2 \rceil = (b^2+3)/2$. The case $b = 3$ can be checked directly, we assume that $b \geqslant 5$. Consider vertices $2b$ and x. From the structure of G^b, it is easy to see that $k_{2b,x}(G^b) > (b-1)/2$, hence, $k_{2b,x}(G) > (b^2-b)/2$. Furthermore, let $2b \xrightarrow{\frac{b^2-b}{2}} v_1 \xrightarrow{l} w$, $x \xrightarrow{\frac{b^2-b}{2}} v_2 \xrightarrow{l} w$ in G for some vertex w and $l < (b+3)/2$. Then in G^b we have $2b \xrightarrow{\frac{b-1}{2}} v_1$, $x \xrightarrow{\frac{b-1}{2}} v_2$, $v_1 \xrightarrow{1} \tilde{w}$, $v_2 \xrightarrow{1} \tilde{w}$ for some vertex $\tilde{w}$. There are only two possible situations: $v_1 = (b-3)/2, v_2 = (b-1)/2$ or $v_1 = (b-3)/2, v_2 = x$.

In the first situation, we obtain $k_{v_1,v_2}(G) = (b-1)/2 + k_{b-1,b-2}(G) = (b+3)/2$.

If the second situation holds, then $k_{v_1,v_2}(G) = (b+1)/2 + k_{b-1,b}(G) = (b+3)/2$.

Thus in both situations $k_{2b,x}(G) \geqslant (b^2-b)/2 + (b+3)/2 = (b^2+3)/2$, as required.

If $n > 2b$, then $k_{n,x}(G) = n - 2b + k_{2b,2b-\lfloor b/2 \rfloor}(H_{2b,b} \cup \{(b+1, 2b)\}) = n - b + \lceil ((b-1)^2+1)/2 \rceil$, as required.

Example 5.6: Let us show that Theorem 1.7 does not hold for arbitrary digraphs. Let $n = m+s$, where s is fixed, m is much greater than s. Let G_1 be an elementary cycle of order s and G_2 equal W_m. Let G be a digraph of order n contained G_1 and G_2 as non-intersected subgraphs connected with some edges from G_1 to G_2. Since G_2 is primitive and reachable in G, by Theorem 4.1 it holds that $k(G) \neq 0$. G has $(G_1 \to G_2)$-partition, hence by Lemma 3.5, Item 1 we have that $k(G) \geqslant k(G_2) = \lceil ((m-1)^2+1)/2 \rceil$.

It is clear that $\lceil ((m-1)^2+1)/2 \rceil \sim m^2/2$ whenever $m \to \infty$. On the other hand,

$$K(n,s) = K(m+s,s) = m + k(m+s,s) = m + \begin{cases} \left(\dfrac{s-1}{2}\right)(m+s), & \text{if } s \text{ is odd;} \\ \left(\dfrac{m+s-1}{2}\right)s, & \text{if } s \text{ is even.} \end{cases}$$

Hence as $m \to \infty$,

$$K(n,s) \sim m + \begin{cases} \dfrac{m(s-1)}{2}, & \text{if } s \text{ is odd;} \\ \dfrac{ms}{2}, & \text{if } s \text{ is even.} \end{cases}$$

Clearly, for sufficiently large m, we obtain that $k(G) \geqslant k(G_2) = \lceil \frac{(m-1)^2+1}{2} \rceil > K(n,s)$, although the girth of G equals s. Thus Theorem 1.7 does not remain true for arbitrary digraphs.

However, the following theorem generalizes Theorem 1.7 in some way.

Theorem 5.7: *Let G be a not strongly connected digraph of order n with $k(G) \neq 0$. Consider its canonical $(G_1 \to G_2)$-partition. Let s be the girth of G_2. Then*

$$k(G) \leqslant 1 + K(n-1,s).$$

If the equality holds, then $|G_2| = n-1$ and $k(G_2) = K(n-1,s)$. Particularly, $k(G) < K(n,s)$.

Proof: G_2 is primitive due to Corollary 3.11. Let $|G_2| = b \leqslant n-1$, $|G_1| = n-b$. From Theorem 1.7, it follows that

$$k(G_2) \leqslant K(b,s) = b - s + k(b,s).$$

Therefore by Lemma 3.5, Item 4, we have

$$\begin{aligned} k(G) &\leqslant |G_1| + k(G_2) = n - b + k(G_2) \leqslant n - s + k(b,s) \\ &\leqslant n - s + k(n-1,s) = 1 + K(n-1,s), \end{aligned} \tag{9}$$

since it is straightforward to see that the function $k(n,s)$ strictly increases with respect to the first argument.

Now let us assume that the equality holds. Then (9) becomes a chain of equalities. Hence, $k(b,s) = k(n-1,s)$. This means that $|G_2| = b = n-1$ and $|G_1| = n-b = 1$. Since $n - b + k(G_2) = 1 + K(n-1,s)$, we have that $k(G_2) = K(n-1,s)$.

Note that $k(G) < K(n,s)$, since $1 + K(n-1,s) < K(n,s)$. Indeed,

$$K(n,s) - (K(n-1,s)+1) = k(n,s) - k(n-1,s) > 0.$$

■

Note that in [8] all primitive digraphs of order n with the girth s and the maximum possible scrambling index $K(n,s)$ (by Theorem 1.7) are described.

6. General bounds for the scrambling index

Theorem 6.1: *Let G be a not strongly connected digraph of order $n \geqslant 3$. Then*

$$k(G) \leqslant 1 + \left\lceil \frac{(n-2)^2+1}{2} \right\rceil. \tag{10}$$

When $n \geqslant 4$, equality holds if and only if $G \cong H_{n,n-1}$.

Proof: Without loss of generality, we assume that $k(G) \neq 0$. Consider the canonical $(G_1 \to G_2)$-partition of G.

Then by Theorem 5.7, $k(G) \leqslant 1 + K(n-1,s)$, where s is the girth of G_2.

Now we claim that $K(n-1,s) \leqslant K(n-1,s+1)$ whenever $s \leqslant n-2$. Indeed,

$$\begin{aligned}
K(n-1,s+1) - K(n-1,s) &= -1 + k(n-1,s+1) - k(n-1,s) \\
&= -1 + \begin{cases} \dfrac{n-2}{2}(s+1) - \dfrac{s-1}{2}(n-1), & \text{when } s \text{ is odd;} \\ \dfrac{s}{2}(n-1) - \dfrac{n-2}{2}s, & \text{when } s \text{ is even} \end{cases} \\
&= -1 + \begin{cases} \dfrac{2n-s-3}{2}, & \text{when } s \text{ is odd;} \\ \dfrac{s}{2}, & \text{when } s \text{ is even.} \end{cases}
\end{aligned}$$

In the case s is even, one obtains $s/2 - 1 \geqslant 0$ with the equality only if $s=2$.

In the case s is odd, one obtains (while $s \leqslant n-2$)

$$-1 + \frac{2n-s-3}{2} = \frac{2n-s-5}{2} \geqslant \frac{2n-(n-2)-5}{2} = \frac{n-3}{2} \geqslant 0$$

with the equalities only if $n=3$, $s=1$.

This implies that

$$\begin{aligned}
k(G) &\leqslant 1 + K(n-1,s) \leqslant 1 + K(n-1,s+1) \leqslant \cdots \leqslant 1 + K(n-1,n-2) \\
&= 1 + \left\lceil \frac{(n-2)^2+1}{2} \right\rceil. \qquad (11)
\end{aligned}$$

Now let us assume that the equality holds. Then by (11), $k(G) = 1 + K(n-1,s)$, therefore by Theorem 5.7 it follows that $|G_2| = n-1$. Moreover, equality at (10) implies that the equality in the statement of Theorem 5.4 holds. Hence by Theorem 5.4, Item 3 it holds that $G \cong H_{n,n-1}$, since $4 \leqslant n < 2(n-1)$. This completes the proof. ■

Remark 6.2: Considering all the digraphs of order 3, it is routine to check that in the case $n=3$ if for a not strongly connected digraph G we have

$$k(G) = 1 + \left\lceil \frac{(n-2)^2+1}{2} \right\rceil = 2,$$

then G is isomorphic to $H_{3,2}$, or $H_{3,2} \cup \{(3,3)\}$, or to any digraph with the vertex set $\{1,2,3\}$ and the edge set $\{(1,1),(2,1),(3,2)\} \cup E$, where $E \subseteq \{(3,3),(2,2),(2,3)\}$.

We can also characterize not strongly connected digraphs with the closest to the maximum value of the scrambling index. For this, we define a set $\mathscr{R}_n$ of digraphs:

$$\begin{aligned}
&G \in \mathscr{R}_n \quad \text{iff} \quad G \cong G' \quad \text{such that } V(G') = \{1,\ldots,n\}, \\
&E(G') = E(W_{n-1}) \cup A, \text{ where } A \subseteq \{(n,i) \mid i = 1,\ldots,n-1\} \cup \{(n,n)\}, \qquad (12) \\
&A \neq \emptyset, \{(n,n-1)\}, \{(n,n)\}.
\end{aligned}$$

Define also a digraph H'_n with the vertex set $\{1,2,\ldots,n\}$ and the edge set $E(W'_{n-1}) \cup \{(n,1)\}$.

Lemma 6.3: *Let $n \geqslant 4$ and $G \in \mathscr{R}_n$ or $G \cong H'_n$. Then $k(G) = \lceil ((n-2)^2+1)/2 \rceil$.*

Proof: If $G \in \mathscr{R}_n$, then $G \cong G'$, where $V(G') = \{1, 2, \ldots, n\}$, $E(G') = E(W_{n-1}) \cup A$ (see (12)). By the definition of $\mathscr{R}_n$ it follows that W_{n-1} is reachable in G', therefore by Theorem 4.1, $k(G') \neq 0$. By Lemma 3.5, Item 1, we have $k(G') \geqslant k(W_{n-1}) = \lceil ((n-2)^2+1)/2 \rceil$.

If $G = H'_n$, then similarly $k(G) \neq 0$. Furthermore, $k_{n,\lfloor (n-1)/2 \rfloor}(H'_n) = 1 + k_{1,\lfloor (n-1)/2 \rfloor+1}(W'_{n-1}) = \lceil ((n-2)^2+1)/2 \rceil$, as follows from Proposition 2.8, Item 1.

Furthermore, in both cases $G \ncong H_{n,n-1}$, hence by Theorem 6.1, one obtains that $k(G) < 1 + \lceil ((n-2)^2+1)/2 \rceil$. Thus $k(G) = \lceil ((n-2)^2+1)/2 \rceil$. ■

Theorem 6.4: *Let G be a not strongly connected digraph of order $n \geqslant 8$. Then $k(G) = \lceil ((n-2)^2+1)/2 \rceil$ if and only if $G \in \mathscr{R}_n$ or $G \cong H'_n$.*

Proof: Let $k(G) = \lceil ((n-2)^2+1)/2 \rceil$. Consider the canonical $(G_1 \to G_2)$-partition of G. From Corollary 3.11, it follows that G_2 is primitive. Let s be the girth of G_2. Obviously, $s < |G_2| \leqslant n-1$. Consider the following two cases:

Case 1. $s \leqslant n-3$. Then, according to the proof of Theorem 6.1 (see (11)), we have

$$k(G) \leqslant 1 + K(n-1, s) \leqslant 1 + K(n-1, s+1) \leqslant \cdots \leqslant 1 + K(n-1, n-3).$$

Note that

$$K(n-1, n-2) - K(n-1, n-3) = -1 + \begin{cases} \frac{n}{2}, & \text{if } n \text{ is even;} \\ \frac{n-3}{2}, & \text{if } n \text{ is odd} \end{cases}$$

and since $n \geqslant 8$, we get $1 < K(n-1, n-2) - K(n-1, n-3)$.

Therefore,

$$k(G) \leqslant 1 + K(n-1, n-3) < K(n-1, n-2) = \left\lceil \frac{(n-2)^2+1}{2} \right\rceil.$$

A contradiction is obtained.

Case 2. $s = n-2$. In this case, $|G_2| = n-1$. Let $V(G_1) = \{n\}$. Note that

$$G_2 \cong W_{n-1} \text{ or } G_2 \cong W'_{n-1}.$$

Subcase 2.1. $G_2 \cong W'_{n-1}$. Suppose that G_2 has the same labelling of vertices as W'_{n-1}. Consider a pair of vertices (u, v), $u > v$ such that $k_{u,v}(G) = k(G) = \lceil ((n-2)^2+1)/2 \rceil$. If $u \neq n$, then $k_{u,v}(G) = k_{u,v}(W'_{n-1}) = \lceil ((n-2)^2+1)/2 \rceil - 1$, a contradiction. Therefore, $u = n$.

It is clear that G does not contain any edges of type (j, n), where $j \neq n$, since G_2 is a strongly connected component of G. However, G contains at least one edge of type (n, i), where $i \neq n$, since G_2 is reachable. Assume that $i \neq 1$.

If $v \neq n-1$, then $k(G) = k_{n,v}(G) \leqslant 1 + k_{i,v+1}(W'_{n-1})$. Therefore, $k_{i,v+1}(W'_{n-1}) = \lceil ((n-2)^2+1)/2 \rceil - 1$ and by Proposition 2.8, Item 2, $1 \in \{i, v+1\}$, a contradiction.

If $v = n-1$, then $k(G) = k_{n,v}(G) \leqslant 1 + k_{i,2}(W'_{n-1})$. Therefore, $k_{i,2}(W'_{n-1}) = \lceil ((n-2)^2+1)/2 \rceil - 1$ and again $1 \notin \{i, 2\}$, a contradiction with Proposition 2.8, Item 2.

This means that $i = 1$ and $G \cong H'_n$ or $G \cong H'_n \cup \{(n,n)\}$. Now let us consider the digraph $H'_n \cup \{(n,n)\}$. We notice that for an arbitrary vertex with the number $l \neq n$, we have $l \xrightarrow{n-l} 1$ and $n \xrightarrow{n-l} 1$. Therefore, since $n \geqslant 8$,

$$k_{n,l}(H'_n \cup \{(n,n)\}) \leqslant n - l \leqslant n - 1 < \frac{(n-2)^2+1}{2} \leqslant \left\lceil \frac{(n-2)^2+1}{2} \right\rceil.$$

From the above and by Corollary 2.4, we get that $k(H'_n \cup \{(n,n)\}) < \lceil ((n-2)^2+1)/2 \rceil$. Thus the only possibility is $G \cong H'_n$.

Subcase 2.2. $G_2 \cong W_{n-1}$. By Corollary 3.11, G_2 is reachable, hence there is an edge from n to some vertex of G_2 in G. However, there is no edge of type (i, n), where $i < n$, since G is not strongly connected. Moreover, $G \ncong H_{n,n-1}$ by Lemma 5.3. Thus the only possibility is $G \in \mathscr{R}_n$ as follows from the definition of this set.

The sufficiency condition follows by Lemma 6.3. ■

The following theorem generalizes Theorem 1.8.

Theorem 6.5: *Let G be an arbitrary digraph of order $n \geqslant 3$. Then*

$$k(G) \leqslant \left\lceil \frac{(n-1)^2+1}{2} \right\rceil.$$

Equality holds if and only if $G \cong W_n$.

Proof: It is sufficient to assume that $k(G) \neq 0$.

Let G be not strongly connected. From Theorem 6.1, we have

$$k(G) \leqslant 1 + \left\lceil \frac{(n-2)^2+1}{2} \right\rceil \leqslant \frac{n^2-4n+8}{2} < \frac{n^2-2n+2}{2} \leqslant \left\lceil \frac{(n-1)^2+1}{2} \right\rceil,$$

while $n \geqslant 4$. If $n = 3$, then

$$k(G) \leqslant 1 + \left\lceil \frac{(n-2)^2+1}{2} \right\rceil = 2 < 3 = \left\lceil \frac{(n-1)^2+1}{2} \right\rceil.$$

This implies that $k(G) < \lceil ((n-1)^2+1)/2 \rceil$ unless G is strongly connected.

Otherwise, G is strongly connected. Hence by Theorem 3.1, G is primitive. Thus Theorem 1.8 states that $k(G) \leqslant \lceil ((n-1)^2+1)/2 \rceil$ and the equality holds if and only if $G \cong W_n$. This completes the proof. ■

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References

[1] Brualdi RA, Ryser HJ. Combinatorial matrix theory. Cambridge: Cambridge University Press; 1991. (Encyclopedia of mathematics and its applications; 39).
[2] Dolinar G, Guterman A, Kuzma B, et al. Double centralizing theorem with respect to q-commutativity relation. J Algebra Appl. 2019;18(01):1950003.
[3] Paz A. Introduction to probabilistic automata. New York: Academic Press; 1971.
[4] Seneta E. Nonnegative matrices and Markov chains. New York: Springer-Verlag; 1981.
[5] Akelbek M. A joint neighbour bound for primitive digraphs [Ph.D. Thesis]. University of Regina; 2008
[6] Akelbek M, Fital S, Shen J. A bound on the scrambling index of a primitive matrix using Boolean rank. Linear Algebra Appl. 2009;431:1923–1931.
[7] Akelbek M, Kirkland S. Coefficients of ergodicity and scrambling index. Linear Algebra Appl. 2009;430:1111–1130.
[8] Akelbek M, Kirkland S. Primitive digraphs with the largest scrambling index. Linear Algebra Appl. 2009;430:1099–1110.
[9] Chen S, Liu B. The scrambling index of symmetric primitive matrices. Linear Algebra Appl. 2010;433:1110–1126.
[10] Guterman AE, Maksaev AM. Additive maps preserving the scrambling index are bijective. Acta Sci Math. 2018;84(1–2):19–38.
[11] Guterman AE, Maksaev AM. Maps preserving matrices of extremal scrambling index. Special Matrices. 2018;6:166–179.
[12] Guterman AE, Maksaev AM. Maps preserving scrambling index. Linear Multilinear Algebra. 2018;66(4):840–851.
[13] Guterman AE, Maksaev AM. Preserving λ-scrambling matrices. Fundamenta Informaticae. 2018;162(2–3):119–141.
[14] Huang Y, Liu B. Generalized scrambling indices of a primitive digraph. Linear Algebra Appl. 2010;433:1798–1808.
[15] Kim H. Scrambling index set of primitive digraphs. Linear Algebra Appl. 2013;439:1886–1893.
[16] Liu B, Huang Y. The scrambling index of primitive digraphs. Comput Math Appl. 2010;60:706–721.
[17] Mulyono SS. The scrambling index of two-colored Wielandt digraph. Universal J Appl Math. 2014;2(6):250–255.
[18] Brualdi RA, Liu B. Generalized exponents of primitive directed digraphs. J Graph Theory. 1990;14:483–499.
[19] Tarjan R. Depth-first search and linear graph algorithms. SIAM J Comput. 1972;1(2):146–160.