



Feedback numbers of de Bruijn digraphs[☆]

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ABSTRACT

A subset of vertices of a graph G is called a feedback vertex set of G if its removal results in an acyclic subgraph. Let $f(d, n)$ denote the minimum cardinality over all feedback vertex sets of the de Bruijn digraph $B(d, n)$. This paper proves that for any integers $d \geq 2$ and $n \geq 2$

$$f(d, n) = \begin{cases} \frac{1}{n} \sum_{i|n} d^i \varphi\left(\frac{n}{i}\right) & \text{for } 2 \leq n \leq 4; \\ \frac{d^n}{n} + O(nd^{n-4}) & \text{for } n \geq 5, \end{cases}$$

where $i | n$ means i divides n , and $\varphi(i)$ is the Euler totient function.

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1. Introduction

Let $G = (V, E)$ be a graph or digraph without multiple edges, with vertex set $V(G)$ and edge set $E(G)$. It is well known that the cycle rank of a graph G is the minimum number of edges that must be removed in order to eliminate all of the cycles in the graph. That is, if G has v vertices, ε edges, and ω connected components, then the minimum number of edges whose deletion from G leaves an acyclic graph equals the cycle rank (or Betti number) $\rho(G) = \varepsilon - v + \omega$.

A corresponding problem is the removal of vertices. A subset $F \subset V(G)$ is called a *feedback vertex set* if the subgraph $G - F$ is acyclic, that is, if $G - F$ is a forest. The minimum cardinality of a feedback vertex set is called the *feedback number* (or *decycling number* proposed first by Beineke and Vandell [1]) of G . A feedback vertex set of this cardinality is called a *minimum feedback vertex set*.

Determining the feedback number of a graph G is equivalent to finding the greatest order of an induced forest of G proposed first by Erdős, Saks and Sós [2], since the sum of the two numbers equals the order of G . A review of recent results and open problems on the decycling number is provided by Bau and Beineke [3].

Apart from its graph-theoretical interest, the minimum feedback vertex set problem has important applications to several fields; for example, in operating systems to resource allocation mechanisms that prevent deadlocks [4], in artificial intelligence to the constraint satisfaction problem and Bayesian inference, in synchronous distributed systems to the study of monopolies and in optical networks to converters' placement problem (see [5,6]).

The minimum feedback set problem is known to be *NP*-hard for general graphs [7] and the best known approximation algorithm is one with an approximation ratio two [8]. Determining the feedback number is quite difficult even for some elementary graphs. However, the problem has been studied for some special graphs and digraphs, such as hypercubes, meshes, toroids, butterflies, cube-connected cycles, directed split-stars (see [5,6,8–16]).

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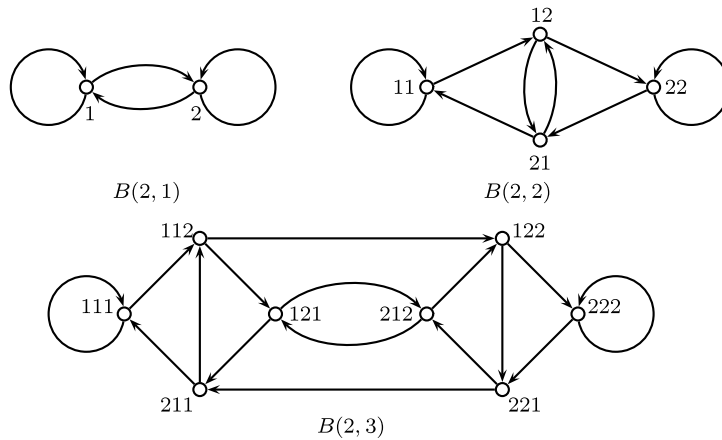


Fig. 1. de Bruijn digraphs $B(2, 1)$, $B(2, 2)$ and $B(2, 3)$.

The de Bruijn digraph $B(d, n)$ has the words of length $n \geq 1$ over an alphabet of size $d \geq 1$ as vertices and there is a directed edge from $x_1x_2 \cdots x_n$ to $y_1y_2 \cdots y_n$ if and only if $y_i = x_{i+1}$ for each $i = 1, 2, \dots, n - 1$. The Kautz digraph $K(d, n)$, $d \geq 2$, is defined as the subdigraph of $B(d + 1, n)$ induced by the words with different consecutive symbols.

As a topological architecture of interconnection networks, the de Bruijn digraph and the Kautz digraph have many attractive features superior to the hypercube, such as it is regular, Eulerian, Hamiltonian, and has small diameter, optimal connectivity, simple recursive structure, simple routing algorithm, contains some other useful topologies as its subgraphs (see, for example, Section 3.3 in [17]) and, thus, been thought of as a good candidate for the next generation of parallel system architectures, after the hypercube network [18].

Králóvič and Růžička [19] proved that the feedback number of the de Bruijn undirected graph $UB(2, n)$, obtained from $B(2, n)$ by deleting the orientation of all edges and omitting multiple edges and loops, is $\lceil \frac{2^n - 2}{3} \rceil$. Recently, Xu et al. [20] have determined the exact values of the feedback number of the Kautz digraph $K(d, n)$ for $1 \leq n \leq 7$ and the asymptotical values for $n \geq 8$.

In this paper, we consider the feedback number of the de Bruijn digraph $B(d, n)$. Use $f(d, n)$ to denote the feedback number of $B(d, n)$. By refining and developing the method in [20], we can show the result as follows. For any integers $d \geq 2$ and $n \geq 2$

$$f(d, n) = \begin{cases} \frac{1}{n} \sum_{i|n} d^i \varphi\left(\frac{n}{i}\right) & \text{for } 2 \leq n \leq 4; \\ \frac{d^n}{n} + O(nd^{n-4}) & \text{for } n \geq 5, \end{cases}$$

where $i | n$ means i divides n , and $\varphi(i)$ is the Euler totient function, that is, $\varphi(1) = 1$ and $\varphi(i) = i \cdot \prod_{j=1}^r \left(1 - \frac{1}{p_j}\right)$ for $i \geq 2$, where p_1, \dots, p_r are the distinct prime factors of i , not equal to 1.

The proof of the result is in Section 3. In Section 2, we give the definition of the de Bruijn digraph $B(d, n)$, construct a feedback vertex set of $B(d, n)$ and gives several lemmas.

2. Feedback vertex sets

In this section, our main aim is to construct two important sets $\Phi(d, n)$ and $F(d, n)$ in $B(d, n)$, respectively, where the former is a set of some cycles in $B(d, n)$ and the latter is a feedback vertex set of $B(d, n)$ for $n \geq 2$, and then to show that the feedback number $f(d, n)$ of $B(d, n)$ satisfies $f(d, n) = |\Phi(d, n)|$ for $2 \leq n \leq 4$ and $|\Phi(d, n)| \leq f(d, n) \leq |F(d, n)|$ for $n \geq 5$. The main idea and methods is essentially due to Xu et al. [20].

Definition 2.1. The de Bruijn digraph $B(d, n)$ ($d \geq 2, n \geq 1$) is defined as follows. The vertex set of $B(d, n)$ is

$$V(d, n) = \{x_1x_2 \cdots x_n : x_i \in \{1, 2, \dots, d\}, 1 \leq i \leq n\}.$$

There are d arcs from one vertex $X = x_1x_2 \cdots x_n$ to d other vertices $Y = x_2x_3 \cdots x_n\alpha$, where $\alpha \in \{1, 2, \dots, d\}$.

The digraphs showed in Fig. 1 are $B(2, 1)$, $B(2, 2)$ and $B(2, 3)$, respectively.

It is clear that the de Bruijn digraph $B(d, n)$ is d -regular and has order d^n . Moreover, $B(d, n)$ has d cycles of length one, i.e. self-loops, each one of them is at the vertex $\underbrace{iii \dots ii}_n$ for each $i = 1, 2, \dots, d$. Let

$$V'(d, n) = \{\underbrace{iii \dots ii}_n \in V(d, n) : i = 1, 2, \dots, d\}.$$

It is clear that $V'(d, n)$ is included in any feedback vertex set of $B(d, n)$ since any vertex in $V'(d, n)$ is incident with a self-loop. Since $B(d, 1)$ is a flowered complete digraph K_d^+ obtained from a complete digraph K_d by appending a self-loop at each vertex, there are no non-trivial feedback vertex sets in K_d^+ . Thus, we assume $n \geq 2$ below.

Definition 2.2. Define a mapping $\phi_n : V(d, n) \rightarrow V(d, n)$ subject to

$$\phi_n(X) = x_2x_3 \cdots x_nx_1, \quad \text{for } X = x_1x_2x_3 \cdots x_n \in V(d, n).$$

It is clear that ϕ_n is a bijective mapping. For any $X = x_1x_2x_3 \cdots x_n \in V(d, n)$, $\phi_n^n(X) = X$, there exists a smallest positive integer t , denoted by $\text{ind}(X)$, such that $\phi_n^t(X) = X$, which means that t divides j for any positive integer j such that $\phi_n^j(X) = X$.

Moreover, $[X]_{\phi_n} = (X, \phi_n(X), \dots, \phi_n^{t-1}(X), X)$ is a directed cycle in $B(d, n)$ for any $X \in V(d, n)$ and is equivalent to $(\phi_n^i(X), \phi_n^{i+1}(X), \dots, \phi_n^{t-1}(X), X, \dots, \phi_n^{i-1}(X), \phi_n^i(X))$ for any integer i with $1 \leq i \leq t - 1$, where $t = \text{ind}(X)$. For short, we will replace $[X]_{\phi_n}$ by $[X]$ in the following discussion. Let

$$\Phi(d, n) = \{ [X] : X \in V(d, n) \}. \tag{2.1}$$

Theorem 2.1. Let F be a minimum feedback vertex set in $B(d, n)$, $d \geq 2$ and $n \geq 2$. Then

$$|F| \geq |\Phi(d, n)| \geq \left\lceil \frac{d^n - d}{n} \right\rceil + d,$$

the equality $|F| = |\Phi(d, n)|$ holds if and only if $|F \cap [X]| = 1$. Moreover, $|\Phi(d, n)| \geq \lceil \frac{d^n - d^2}{n} \rceil + d + \frac{1}{2}d(d - 1)$ if n is even.

Proof. Let F be a minimum feedback vertex set in $B(d, n)$. Then F must contain at least one vertex of every cycle in $\Phi(d, n)$ and, hence, $|F| \geq |\Phi(d, n)|$. It is clear that $|F| = |\Phi(d, n)| \Leftrightarrow |F \cap [X]| = 1$.

It is clear that $[X] = [Y]$ or $[X] \cap [Y] = \emptyset$ for any two cycles $[X]$ and $[Y]$ in $\Phi(d, n)$. Since $B(d, n)$ is $(d - 1)$ strongly connected, each vertex of $B(d, n)$ must lie on a cycle. These two facts mean that the vertex sets of cycles in $\Phi(d, n)$ is a partition of $V(d, n)$. Since d cycles in $\Phi(d, n)$ have length one, which contain d vertices, and otherwise have length at most n , $|\Phi(d, n)| \geq \left\lceil \frac{d^n - d}{n} \right\rceil + d$.

Note that if n is even, let $X = ijij \cdots ijij$ with $i \neq j$, then $[X] \in \Phi(d, n)$ and $\phi_n^2(X) = X$, that is, the length of $[X]$ is two. There are $\frac{1}{2}d(d - 1)$ such cycle $[X]$'s, which contain $d(d - 1)$ vertices for $d \geq 2$ and $n \geq 2$. Thus, $|\Phi(d, n)| \geq \left\lceil \frac{d^n - d^2}{n} \right\rceil + d + \frac{1}{2}d(d - 1)$.

The theorem follows. \square

The lower bound of $f(d, n)$ given in Theorem 2.1 is best possible in view of $B(2, 3)$. For example, see Fig. 1, $f(2, 3) \geq 4$ and $F = \{000, 111, 100, 101\}$ is a feedback vertex set in $B(2, 3)$.

For any integers d and n with $d \geq 2$ and $n \geq 1$, let

$$\Omega_{d,n} = \{x_1x_2 \cdots x_m \in V(d, m) : 1 \leq m \leq n + d^n\},$$

where $d^n = |V(d, n)|$. For any $X = x_1x_2 \cdots x_m \in \Omega_{d,n}$, let $X(i) = x_1x_2 \cdots x_i$, $1 \leq i \leq m$, where m is called the length of X , denoted by $\ell(X)$, i.e., $\ell(X) = m$ and $\ell(X(i)) = i$. We also write $X(i) \subseteq X$ if $i \leq m$ and $X(i) \subset X$ if $i < m$. For $X = x_1x_2 \cdots x_m$, $Y = y_1y_2 \cdots y_\ell \in \Omega_{d,n}$, we write

$$X > Y \Leftrightarrow \sum_{i=1}^m x_i(d + 1)^{m-i} > \sum_{i=1}^{\ell} y_i(d + 1)^{\ell-i}.$$

Clearly, $Y < X$ if $Y \subset X$.

Theorem 2.2. For any fixed integer $d \geq 2$, let F_d be a subset of $\Omega_{d,n}$ satisfying the following conditions:

- (a) $F_d \cap [X] \neq \emptyset$ for any $X \in \Omega_{d,n}$;
- (b) $X(i) \in F_d$ for any $X \in F_d$ and any $X(i) \subset X$.

Then $F_d \cap V(d, n)$ is a feedback set of $B(d, n)$ for any $n \geq 2$.

Proof. Let $F = F_d \cap V(d, n)$ for convenience and suppose to the contrary that $B(d, n) - F$ still contains a directed cycle C of length j ($1 \leq j \leq d^n$):

$$C = (x_1x_2 \cdots x_n, x_2x_3 \cdots x_{n+1}, \dots, x_{n+j-1}x_1 \cdots x_{n-1}, x_1x_2 \cdots x_n).$$

Then $F \cap C = \emptyset$ and there is a sequence $X = x_1x_2 \cdots x_nx_{n+1} \cdots x_{n+j-1} \in \Omega_{d,n}$ with length $\ell = n + j - 1$ and also we can express

$$C = (X(n), \phi_\ell(X)(n), \dots, \phi_\ell^{j-1}(X)(n), X(n)).$$

By the condition (a) there exists an integer k such that $Y = \phi_\ell^k(X) \in F_d \cap [X]$ and $Y(n) \in C$. By the condition (b), $Y(n) \in F_d$, of course, $Y(n) \in V(d, n)$, and so $Y(n) \in F$. Thus $F \cap C \neq \emptyset$, a contradiction, and so $F_d \cap V(d, n)$ is a feedback set of $B(d, n)$. \square

For any integers d and n with $d \geq 2$ and $n \geq 2$, let

$$\Omega'_{d,n} = \{x_1x_2 \cdots x_m \in \Omega_{d,n} : m \geq 2, x_1 > x_2, x_1 \geq x_i, 3 \leq i \leq m\}.$$

Let $X = x_1x_2 \cdots x_m \in \Omega'_{d,n}$, $p = x_1$ and let p^t denote the sequence $\underbrace{pp \cdots p}_t$. Then we can write X as

$$X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r \quad \text{or} \quad X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r p^{t_{r+1}}, \tag{2.2}$$

where X_i is a non-empty sub-sequence of X between p^{t_i} and $p^{t_{i+1}}$ and each digit in X_i is less than p , $1 \leq t_i \leq n - 2$ and $2 \leq i \leq r + 1$.

For example, let $X = 72177721772 \in \Omega'_{7,11}$, then $p = 7$ and X can be expressed as $7X_17^3X_27^2X_3$, where $X_1 = X_2 = 21$ and $X_3 = 2$. $[X] \cap \Omega'_{7,11} = \{X, \phi^5(X), \phi^9(X)\}$.

Definition 2.3. For any integers d and n with $d \geq 2$ and $n \geq 2$, define

$$F(d, n) = F_d \cap V(d, n), \tag{2.3}$$

where $F_d \subset \Omega'_{d,n} \cup V'(d, n)$ such that each $X \in F_d$ satisfies one of the following forms:

- (1) $X = p^n$;
- (2) $X = \underbrace{pX_1p^{t_2}X_1p^{t_3} \cdots p^{t_r}X_1}_r$, or $X = \underbrace{pX_1p^{t_2}X_1p^{t_3} \cdots p^{t_r}X_1}_{r+1} p^{t_{r+1}}$, $r \geq 1$;
- (3) $X = \underbrace{pX_1p^{t_2}X_1p^{t_3} \cdots p^{t_{r-1}}X_1}_{r-1} p^{t_r}X_r$, $r \geq 3$ and $X_r \subset X_1$;
- (4) $X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r$, or $X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r p^{t_{r+1}}$, $r \geq 2, X_1 > X_2, X_1 \geq X_i, i = 3, \dots, r$.

For example, $\{71217121, 71271271, 71271712\} \subset F_7$, in which the vertices satisfy the forms (2), (3) and (4), respectively. But $71271272 \notin F_7$ because $71271272 = 7X_17X_17X_2$ and $X_2 \not\subset X_1(1)$, which does not satisfy any form in Definition 2.3.

Theorem 2.3. The set $F(d, n)$ defined in (2.3) is a feedback set of $B(d, n)$ for $n \geq 2$.

Proof. We only need to prove that F_d defined in Definition 2.3 satisfies both the conditions (a) and (b) in Theorem 2.2.

(a) We need to check that $F_d \cap [Y] \neq \emptyset$ for any $Y \in \Omega_{d,n}$. Let $Y = x_1x_2 \cdots x_m$ be any element in $\Omega_{d,n}$. If $x_1 = x_2 = \cdots = x_m = p$, then Y satisfies the form (1) in Definition 2.3, and so $Y \in F_d$ clearly. Otherwise, there exists an integer k such that $x_k = \max\{x_i : 1 \leq i \leq m\}$ with $x_{k+1} < x_k$, where the subscript $k + 1$ is taken modulo m . Let $X = \phi_m^{k-1}(Y) = x_kx_{k+1} \cdots x_mx_1x_2 \cdots x_{k-1}$, then $[X] = [Y]$ and $X \in \Omega'_{d,n}$. We only need to prove $F_d \cap [X] \neq \emptyset$ for any $X \in \Omega'_{d,n}$.

Let $X \in \Omega'_{d,n}$. Then X can be expressed as one of two forms in (2.2). Without loss of generality, we only consider the former since the latter does not satisfy the form (3) in Definition 2.3 and the proof is similar and simpler. Let $X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r$, $r \geq 1$.

If $r = 1$, then $X = pX_1$ and satisfies the form (2). Thus, $X \in F_d$, and so $F_d \cap [X] \neq \emptyset$.

If $r = 2$, then $X = pX_1p^{t_2}X_2$. If $X_1 = X_2$, then X satisfies the form (2); if $X_1 > X_2$, then X satisfies the form (4). In the two cases, $X \in F_d$. If $X_1 < X_2$, then $X' = \phi_m^{\ell(X_1)+t_2}(X) = pX_2pX_1p^{t_2-1}$ satisfies the form (4). Thus, $X' \in F_d$ and $F_d \cap [X] \neq \emptyset$.

Assume $r \geq 3$ below. If $X_1 = X_2 = \cdots = X_r$, then X satisfies the form (2) and $[X] \in F_d$. Otherwise there exists an integer j such that $X_j > X_{j+1}$ and $X_j \geq X_i$, $1 \leq i \neq j + 1 \leq r$, where the subscript $j + 1$ is taken modulo r , then

$$X' = \phi_m^k(X) = pX_jp^{j+1}X_{j+1}p^{t_{j+2}} \cdots p^{t_r}X_r pX_1p^{t_2} \cdots p^{t_{j-1}}X_{j-1}p^{t_j-1}$$

satisfies the form (4), where $k = \ell(pX_1p^{t_2} \cdots p^{t_{j-1}}X_{j-1}p^{t_j-1})$, and $X' \in F_d$, that is, $F_d \cap [X] \neq \emptyset$.

(b) We now check that F_d satisfies the condition (b) in Theorem 2.2, that is, $X(i) \in F_d$ for any $X \in F_d$ and any $X(i) \subseteq X$. Let X be any element in F_d . If $X \in V'(d, m)$, then $X(i) \in F_d$ for any $X(i) \subseteq X$, clearly. Assume $X \in \Omega'_{d,n}$ below. Then X can be expressed as one of the forms in (2.2), say, $X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r$, $r \geq 1$. Thus, $X(i) \subset X$ is of one of the following forms:

- $X(i) = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_s}X_s$ or
- $X(i) = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_s}X_s p^{s+1}$ or
- $X(i) = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_s}X'_s$,

where $s \leq r$, $X'_s \subset X_s$. We only need to check that $X(i) = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_s}X'_s$ (the other cases are similar and simpler) satisfies the condition (b) in Theorem 2.2.

For $s = 1$ or 2 , $X(i)$ satisfies the form (2) or (4) in Definition 2.3, respectively, and so $X(i) \in F_d$ obviously. Assume $s \geq 3$ below.

If $X_1 = X_2$ and X only is of either the form (2) or the form (3) in Definition 2.3, we have $X_1 = X_2 = \cdots = X_{s-1} = X_s$ and $X'_s \subset X_s = X_1$. Then $X(i)$ is of the form (3). Otherwise $X_1 \neq X_2$ and X only is of the form (4). We have $X_1 > X_2, X_1 \geq X_j, 3 \leq j \leq s - 1$, and $X_1 \geq X_s > X'_s$. Then $X(i)$ is of the form (4), which also implies $X(i) \in F_d$.

The proof of the theorem is complete. \square

Theorem 2.4. For $2 \leq n \leq 4$, the set $F(d, n)$ defined in (2.3) is a minimum feedback vertex set of $B(d, n)$ and $|F(d, n)| = |\Phi(d, n)|$.

Proof. We only need to prove that $|F(d, n) \cap [X]| = 1$ for any vertex $X \in V(d, n)$ by Theorems 2.1 and 2.3.

Let $Y = x_1x_2 \dots x_n$ be any element in $V(d, n)$. If $x_1 = x_2 = \dots = x_n = p$, then Y satisfies the form (1) in Definition 2.3, and so $Y \in F_d$ and $|F(d, n) \cap [X]| = 1$ clearly. Otherwise, there exists an integer k such that $x_k = \max\{x_i : 1 \leq i \leq n\}$ with $x_{k+1} < x_k$, where the subscript $k + 1$ is taken modulo n . Let $X = \phi_n^{k-1}(Y) = x_kx_{k+1} \dots x_nx_1x_2 \dots x_{k-1}$, then $[X] = [Y]$ and $X \in \Omega'_{d,n}$. We only need to prove $F_d \cap [X] \neq \emptyset$ for any $X \in \Omega'_{d,n} \cap V(d, n)$.

Let $X \in \Omega'_{d,n} \cap V(d, n)$. Then X can be expressed as one of two forms in (2.2). Assume, without loss of generality, $X = pX_1p^{t_2}X_2p^{t_3} \dots p^{t_r}X_r \in V(d, n)$ (the case $X = pX_1p^{t_2}X_2p^{t_3} \dots p^{t_r}X_r p^{t_{r+1}}$ is similar). The proof depends on the form of F_d , as defined in Definition 2.3, that X satisfied.

If X satisfies the form (2), then it is easy to verify that $F(d, n) \cap [X] = \{X\}$ when $r = 1$. Assume $r \geq 2$ below. Then $X = px_2px_2$ since $n \leq 4$. Clearly, $F(d, n) \cap [X] = \{X\}$.

If X satisfies the form (3), then $X_1 = X_2$ and $X_3 = X_1(i)$, where $i = \ell(X_3) < \ell(X_1)$. Thus, $n \geq 3 + 2(i + 1) + i \geq 8$, which contradicts our hypothesis $n \leq 4$.

If X satisfies the form (4), then $n \geq 4$, that is, $X = px_1px_4$. Thus, $F(d, n) \cap [X] \subseteq \{px_2px_4, px_4px_2\}$. Since $x_2 > x_4$, px_4px_2 does not satisfy the form (4), and so $|F(d, n) \cap [X]| = 1$.

The proof of the theorem is complete. \square

3. Bounds of feedback number

In the preceding section, we construct two important sets $\Phi(d, n)$ and $F(d, n)$ defined in (2.1) and (2.3), respectively. By Theorems 2.1–2.4, we have that

$$f(d, n) = |\Phi(d, n)| \quad \text{for } 2 \leq n \leq 4; \\ \left\lceil \frac{d^n - d}{n} \right\rceil + d \leq |\Phi(d, n)| \leq f(d, n) \leq |F(d, n)| \quad \text{for } n \geq 5. \tag{3.1}$$

In this section, we determine the value of $|\Phi(d, n)|$ and establish an upper bound of $|F(d, n)|$ for $n \geq 5$. The value of $|\Phi(d, n)|$ is expressed in terms of the well-known Euler totient function $\varphi(i)$, that is,

$$\varphi(i) = \begin{cases} 1 & \text{if } i = 1; \\ i \cdot \prod_{j=1}^r \left(1 - \frac{1}{p_j}\right) & \text{if } i \geq 2, \end{cases}$$

where p_1, \dots, p_r are the distinct prime factors of i , not equal to 1.

Lemma 3.1. Let $d \geq 2$ be a fixed integer. Then for any integer $n \geq 2$,

$$|\Phi(d, n)| = \frac{1}{n} \sum_{i|n} d^i \varphi\left(\frac{n}{i}\right), \quad \text{where } i | n \text{ means } i \text{ divides } n.$$

Proof. If we regard a self-loop in $B(d, n)$ as a cycle of length one, then the set $\{[X] : X \in V(d, n)\}$ corresponds to the set of cyclical multiple permutations of length n on the set of d elements, whose total number is (see, for example, [21] or [22])

$$\frac{1}{n} \sum_{i|n} d^i \varphi\left(\frac{n}{i}\right).$$

It follows immediately that

$$|\Phi(d, n)| = |\{[X] : X \in V(d, n)\}| = \frac{1}{n} \sum_{i|n} d^i \varphi\left(\frac{n}{i}\right).$$

The lemma follows. \square

Let

$$E(d, n) = \{X \in F(d, n) : |F(d, n) \cap [X]| \geq 2\}. \tag{3.2}$$

For $2 \leq n \leq 4$, it is clear from Theorem 2.4 that $E(d, n) = \emptyset$, and for $n \geq 5$

$$|F(d, n)| \leq |\Phi(d, n)| + |E(d, n)| \tag{3.3}$$

since $F(d, n) - E(d, n) = \{X \in F(d, n) : |F(d, n) \cap [X]| = 1\} \subseteq \Phi(d, n)$.

For example, in $F(2, 5)$ we have $[21212] = [21221]$ and $\{21212, 21221\} \subseteq E(2, 5)$.

Lemma 3.2. Let $d \geq 2$ be a fixed integer. Then for any integer $n \geq 5$,

$$|E(d, n)| \leq \frac{n^2}{n-4} d^{n-4} = O(nd^{n-4}).$$

Proof. Suppose $X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r$ or $X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_r}X_r p^{r+1} \in E(d, n)$, where $2 \leq p \leq d$ and $1 \leq r \leq \frac{n}{2}$.

We first note that $[X] \cap F(d, n) = \{X\}$ if X is of the form (4) in Definition 2.3 with $r = 2$. In fact, if $X = pX_1p^{t_2}X_2$ or $X = pX_1p^{t_2}X_2p^{t_3}$ with $X_1 > X_2$, then $[X] \cap F(d, n) = \{X\}$ by the restrictive condition $X_1 > X_2$.

Suppose that X is of the form (2). If $r = 1$ or $t_2 = t_3 = \cdots = t_r = 1$, then $[X] \cap F(d, n) = \{X\}$, clearly. Otherwise, $r \geq 2$ and $1 + t_2 + t_3 + \cdots + t_r > r$. Then

$$[X] \cap F(d, n) = \{pX_1p^{t_2}X_1p^{t_3}X_1 \cdots p^{t_r}X_1, pX_1p^{t_3}X_1 \cdots p^{t_r}X_1pX_1p^{t_2-1}, \dots, pX_1pX_1p^{t_2}X_1p^{t_3}X_1 \cdots p^{t_{r-1}}X_1p^{t_r-1}\}.$$

For a given integer p with $2 \leq p \leq d$, let

$$E_1(p, n) = \{pX_1p^{t_2}X_1p^{t_3}X_1 \cdots p^{t_r}X_1, pX_1p^{t_3}X_1 \cdots p^{t_r}X_1pX_1p^{t_2-1}, \dots, pX_1pX_1p^{t_2}X_1p^{t_3}X_1 \cdots p^{t_{r-1}}X_1p^{t_r-1} \in F(d, n) : t_2 + t_3 + \cdots + t_r \geq r, r \geq 2\}.$$

To estimate $|E_1(p, n)|$, let $j = \ell(X_1)$, $X' = p^{t_4}X_1p^{t_5}X_1 \cdots p^{t_r}X_1$ and $\ell(X') = n - 1 - t_2 - t_3 - 3j$. Because $n - rj \geq r + 1$, $1 \leq j \leq \lfloor \frac{n-r-1}{r} \rfloor$. There are $(p - 1)^j$ ways to choose X_1 , $p^{n-1-t_2-t_3-3j}$ ways to choose X' since any digit in X' comes from $\{1, 2, \dots, p\}$, and there are at most $\binom{n-3j-2}{2-1} = n - 3j - 1$ ways to choose $\{t_2, t_3\}$. Thus, it is not difficult to get that

$$\begin{aligned} |E_1(d, n)| &\leq r \sum_{j=1}^{\lfloor \frac{n-r-1}{r} \rfloor} (p - 1)^j p^{n-1-t_2-t_3-3j} (n - 3j - 1) \\ &\leq r \sum_{j=1}^{\lfloor \frac{n-r-1}{r} \rfloor} np^j p^{n-1-t_2-t_3-3j} = r \sum_{j=1}^{\lfloor \frac{n-r-1}{r} \rfloor} np^{n-1-t_2-t_3-2j} \\ &\leq n^2 p^{n-1-t_2-t_3-2}. \end{aligned}$$

Noting $1 + t_2 + t_3 \geq 3$, we have

$$|E_1(d, n)| \leq n^2 p^{n-5}. \tag{3.4}$$

We now consider X that is of the form (3) or (4) in Definition 2.3. Then $r \geq 3$.

Assume $r = 3$. If X is of the form (3), then $X = pX_1p^{t_2}X_1p^{t_3}X_2$, where $X_2 \subset X_1$. It is easy to verify that

$$F(d, n) \cap [X] = \{pX_1p^{t_2}X_1p^{t_3}X_2, pX_1p^{t_3}X_2pX_1p^{t_2-1}\},$$

where the first element is of the form (3) and the second is of the form (4). If X is of the form (4), then $X = pX_1p^{t_2}X_2p^{t_3}X_3$ or $X = pX_1p^{t_2}X_2p^{t_3}X_3p^{t_4}$, where $X_1 > X_2$ and $X_1 \geq X_3$. It is also easy to verify that if $X_1 \neq X_3$ or $X_1 = X_3$ but $t_3 = 1$, then $F(d, n) \cap [X] = \{X\}$; if $X_1 = X_3$ and $t_3 \geq 2$, then $F(d, n) \cap [X] = \{pX_1p^{t_2}X_2p^{t_3}X_1, pX_1p^{t_2}X_2pX_1p^{t_3-1}\}$. For a given integer p with $2 \leq p \leq d$, let

$$E_2(p, n) = \{pX_1p^{t_2}X_2p^{t_3}X_1, pX_1p^{t_2}X_2pX_1p^{t_3-1} \in F(d, n)\}.$$

Let $j = \ell(X_1)$. Then there are at most $(p - 1)^j$ ways to choose X_1 in $E_2(p, n)$. Let $h = 1 + t_2 + t_3$ with $t_3 \geq 2$. Then $4 \leq h \leq n - 2j - 1$ since $\ell(X_2) = n - 2j - h \geq 1$, that is, $1 \leq j \leq \frac{n-5}{2}$. There are at most $\binom{n-2j-3}{2-1} = n - 2j - 3$ ways to choose $\{t_2, t_3\}$, and at most $(p - 1)^{n-2j-h}$ ways to choose X_2 . Thus,

$$\begin{aligned} |E_2(p, n)| &\leq 2 \sum_{j=1}^{\lfloor \frac{n-5}{2} \rfloor} (p - 1)^j (p - 1)^{n-2j-h} (n - 2j - 3) \\ &\leq 2 \sum_{j=1}^{\lfloor \frac{n-5}{2} \rfloor} n(p - 1)^{n-j-4} \leq n^2 p^{n-5}, \end{aligned}$$

that is,

$$|E_2(p, n)| \leq n^2 p^{n-5}. \tag{3.5}$$

Assume $r \geq 4$ below. It is clear that $X_1 \geq X_i$ for $i = 3, 4, \dots, r - 1$. If $X_1 > X_i$ for each $i = 3, 4, \dots, r - 1$, then $[X] \cap F(d, n) = \{X\}$. Otherwise, there must exist some integer i with $3 \leq i \leq r - 1$ such that $X_i = X_1$. Then

$$X = pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_{i-1}}X_{i-1}p^{t_i}X_1p^{t_{i+1}}X_{i+1}p^{t_{i+2}} \cdots p^{t_r}X_r.$$

Thus, $\{X, \phi_n^\ell(X)\} \subset [X] \cap F(d, n)$, where $\ell = \ell(pX_1p^{t_2}X_2p^{t_3} \cdots p^{t_{i-1}}X_{i-1}p^{t_i-1})$.

For a given integer p with $2 \leq p \leq d$, let

$$E_3(p, n) = \{pX_1p^{t_2} \cdots p^{t_{i-1}}X_{i-1}pX_1p^{t_{i+1}}X_{i+1}p^{t_{i+2}} \cdots p^{t_r}X_r(p^{t_{r+1}}) \in F(d, n) : 3 \leq i \leq r-1\}.$$

To estimate $|E_3(p, n)|$, let $j = \ell(X_1)$, $X' = X_2p^{t_3}X_3p^{t_4} \cdots p^{t_{i-1}}X_{i-1}p^{t_{i-1}}$ and $k = \ell(X')$. Then $4 \leq k \leq n-5-2j$. There are $(p-1)^j$ ways to choose X_1 , p^k ways to choose X' since any digit in X' comes from $\{1, 2, \dots, p\}$, $p^{n-4-2j-k}$ ways to choose X_r . Thus, it is not difficult to get that

$$\begin{aligned} |E_3(d, n)| &\leq \sum_{j=1}^{\lfloor \frac{n-6}{2} \rfloor} \sum_{k=4}^{n-5-2j} (p-1)^j p^k p^{n-4-2j-k} \leq \sum_{j=1}^{\lfloor \frac{n-6}{2} \rfloor} \sum_{k=4}^{n-5-2j} p^{n-4-j} \\ &\leq \sum_{j=1}^n p^{n-4-j} (n-2j-8) \leq n^2 p^{n-5}, \end{aligned}$$

that is,

$$|E_3(d, n)| \leq n^2 p^{n-5}. \quad (3.6)$$

It holds clearly that

$$E(d, n) \subseteq \bigcup_{p=2}^d (E_1(p, n) \cup E_2(p, n) \cup E_3(p, n)). \quad (3.7)$$

Thus, by (3.4)–(3.7), we have

$$\begin{aligned} |E(d, n)| &\leq \sum_{p=2}^d (|E_1(p, n)| + |E_2(p, n)| + |E_3(p, n)|) \\ &\leq \sum_{p=2}^d n^2 p^{n-5} = n^2 \sum_{i=1}^{d-1} (i+1)^{n-5}. \end{aligned}$$

Noting that

$$\sum_{i=1}^{d-1} (i+1)^{n-5} \leq \int_0^{d-1} (x+1)^{n-5} dx \leq \frac{d^{n-4}}{n-4},$$

we have $|E(d, n)| \leq \frac{n^2 d^{n-4}}{n-4} = O(nd^{n-4})$, and so the lemma follows. \square

Theorem 3.1. Let $d \geq 2$ be a fixed integer. Then for any integer $n \geq 2$,

$$f(B(d, n)) = \begin{cases} \frac{1}{n} \sum_{i|n} d^i \varphi\left(\frac{n}{i}\right) & \text{for } 2 \leq n \leq 4; \\ \frac{d^n}{n} + O(nd^{n-4}) & \text{for } n \geq 5. \end{cases}$$

Proof. By (3.1), we only need to prove that

$$f(d, n) \leq \frac{d^n}{n} + O(nd^{n-4}) \quad \text{for } n \geq 5. \quad (3.8)$$

Let k be the biggest non-trivial factor of n . Then $k \leq \lfloor \frac{n}{2} \rfloor$ and

$$\sum_{i|n} d^i \varphi\left(\frac{n}{i}\right) = d^n \varphi(1) + O(d^k) = d^n + O(d^k). \quad (3.9)$$

It is from Lemma 3.1 and (3.9) that

$$|\Phi(d, n)| \leq \frac{d^n}{n} + O(nd^{n-4}). \quad (3.10)$$

It follows from (3.1), (3.10) and Lemma 3.2 that

$$f(d, n) \leq |F(d, n)| \leq |\Phi(d, n)| + |E(d, n)| \leq \frac{d^n}{n} + O(nd^{n-4}) \quad \text{for } n \geq 5.$$

The inequality (3.8) holds and the theorem follows. \square

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