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Computation of k-ary Lyndon Words Using Generating Functions and Their Differential Equations

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Abstract. By using generating functions technique, we investigate some properties of the k-ary Lyndon words. We give an explicit formula for the generating functions including not only combinatorial sums, but also hypergeometric function. We also derive higher-order differential equations and some formulas related to the k-ary Lyndon words. By applying these equations and formulas, we also derive some novel identities including the Stirling numbers of the second kind, the Apostol-Bernoulli numbers and combinatorial sums. Moreover, in order to compute numerical values of the higher-order derivative for the generating functions enumerating k-ary Lyndon words with prime number length, we construct an efficient algorithm. By applying this algorithm, we give some numerical values for these derivative equations for selected different prime numbers.

1. Introduction

The Lyndon words arise in many areas of mathematics, computer science and biological sciences. Their potential usage in mathematical modelling have made these words even more attractive to the researchers. Especially, in algebra and algebraic combinatorics there exists various papers on some formulas correspond not only the numbers of these words and related special words, but also dimensions related to free monoid theory and free lie algebra. Moreover, the subject of algorithmic complexity and algorithm desing for generating these words have been studied by many authors in recent years (*cf.* [3, 5, 8, 9, 13–15, 17]; and see also the references cited therein). Generating functions for special numbers and polynomials have been used in almost all braches of mathematics, mathematical pyhsics and other areas. Therefore, because of power of generating functions, in this paper, we modify and unify generating functions for the k-ary Lyndon words including the Apostol-Bernoulli numbers, the Stirling numbers of the second kind and hypergeometric functions. By using these functions, we investigate many properties not only of the generating functions, but also of the k-ary Lyndon words with the help of differential equations and an efficient computational algorithm.

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In order to give our results, we need the following notations and the definitions related to the Lyndon words and some special numbers and polynomials. It is time to give brief definition of the Lyndon words as follows:

The Lyndon word is a lexicographically smallest in its conjugate class which is a set formed by cyclically shifting of the letters in the word. These words are called k-ary Lyndon word of length n if it is derived from the k-letter alphabet Σ and it has n digits (*cf.* [13]). On the other hand, throughout this paper, p denotes a prime number and we investigate properties of the Lyndon words with p prime number length. Note that recently, aperiodic necklaces have been studied as a representative of these words (see [3], [15]; and also the references cited therein). The Figure 1, given by the authors in their recent paper [12], describes how special binary words are represented by a periodic or an aperiodic necklaces.

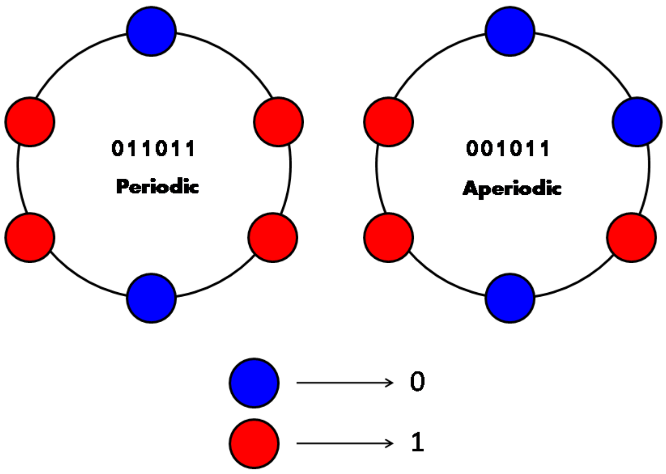

Figure 1: Representing special binary words by a periodic or an aperiodic necklaces.

Let μ be the Möbius function which is defined by

$$\mu(n) = \begin{cases} 1 & n = 1, \\ (-1)^m & \text{if } n \text{ is a square-free integer with } m \text{ distinct prime factors,} \\ 0 & \text{if } n \text{ has a squared prime factor.} \end{cases}$$

(*cf.* [2]). Throughout this paper, we shall be concerned with the polynomials $L_k(n)$ given by

$$L_k(n) = \frac{1}{n} \sum_{d|n} \mu\left(\frac{n}{d}\right) k^d, \tag{1}$$

which enumerating k-ary Lyndon words of length n (*cf.* [3], [15], [13]).

One can easily calculate by equation (1), a few values of the number of k-ary Lyndon words of length n, $L_k(n)$ for $n = 5$ and $k = 1, 2, 3, 4, 5, 6, 7, 8, 9$ is 0, 6, 48, 204, 624, 1554, 3360, 6552, 11808. That is, the number of 6-ary Lyndon words of length 5 is 1554.

The number of k-ary Lyndon words with lenght p^m is given as follows:

$$L_k(p^m) = \frac{k^{p^{m-1}}\left(k^{p^{m-1}(p-1)} - 1\right)}{p^m} \tag{2}$$

(*cf.* [10]).

The generating functions enumerating the k-ary Lyndon words of length p, $f_{L_B}(t,p)$ are defined by the authors in [10] as follows:

$$f_{L_B}(t,p) = \sum_{k=1}^{\infty} L_k(p)\, t^k, \tag{3}$$

where $|t| < 1$.

In [11], the authors also proved the following novel formula for the generating functions $f_{L_B}(t,p)$ in term of the Apostol-Bernoulli numbers $\mathcal{B}_n(t)$, which are given below, by the following theorem:

Theorem 1.1.

$$f_{L_B}(t,p) = \frac{\mathcal{B}_2(t)}{2p} - \frac{\mathcal{B}_{p+1}(t)}{p(p+1)}. \tag{4}$$

Remark 1.2. *The formula (4) is also investigated by Kucukoglu et al. in [12].*

In this paper, by using higher-order derivative of the generating functions $f_{L_B}(t,p)$ in (4), with respect to t, we derive higher-order derivative equations by the following theorems:

Theorem 1.3.

$$\begin{aligned}\frac{d^v}{dt^v}\{f_{L_B}(t,p)\} &= -\frac{1}{p}\frac{(-1)^v v!}{(t-1)^{v+1}}\left[\frac{t+v}{t-1} + \sum_{k=0}^{p} k! S(p,k)\right. \\ &\quad \left.\times \left\{\sum_{j=0}^{v}(-1)^j \binom{v}{j}\binom{k}{j}\frac{1}{(t-1)^j}\left(\frac{t}{1-t}\right)^{k-j}\right\}\right]\end{aligned} \tag{5}$$

where $S(p,k)$ denotes the Stirling numbers of the second kind which are defined in (11).

Theorem 1.4.

$$\begin{aligned}\frac{d^v}{dt^v}\{f_{L_B}(t,p)\} &= -\frac{1}{p}\left[\frac{(-1)^v v!(t+v)}{(t-1)^{v+2}} - \frac{1}{(p+1)(t-1)}\right. \\ &\quad \left.\times \sum_{j=0}^{p}\binom{p+1}{j}\left\{t\frac{d^v}{dt^v}\{\mathcal{B}_j(t)\} + \sum_{k=0}^{v-1}(-1)^{v-k}\frac{v!}{k!(t-1)^{v-k}}\frac{d^k}{dt^k}\{\mathcal{B}_j(t)\}\right\}\right]\end{aligned} \tag{6}$$

where $\mathcal{B}_j(t)$ denotes the Apostol-Bernoulli numbers which are defined in (9).

One of the main motivations of this paper is to derive some novel identities including the Stirling numbers of the second kind, the Apostol-Bernoulli numbers and combinatorial sums related to binomial coefficients using the above theorems. The other motivation is to give some numerical applications of these theorems with their computation algorithm.

Throughout this paper, we also need the following definition, relations and notations:

Let $\mathbb{N} = \{1,2,3,\ldots\}$, $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. $\mathbb{Z}$, $\mathbb{R}$ and $\mathbb{C}$ corresponds the set of integers, the set of real numbers and the set of complex numbers, respectively.

$$0^n = \begin{cases} 1, & n = 0 \\ 0, & n \in \mathbb{N} \end{cases}.$$

Let $m, n \in \mathbb{N}_0$.

$$\binom{m}{n} = \frac{m!}{n!(m-n)!}; 0 \leq n \leq m.$$

If $n < 0$ or $n > m$, then

$$\left(\begin{array}{c} m \\ n \end{array} \right) = 0.$$

For $x \in \mathbb{C}$ and $n \in \mathbb{N}_0$, we have

$$\left(\begin{array}{c} x \\ n \end{array} \right) = \frac{(x)_n}{n!} = \frac{x(x-1)(x-2)\ldots(x-n+1)}{n!},$$

where $(x)_n$ denotes the falling factorial and $(x)_0 = 1$. Also, the rising factorial is given by

$$(x)^{(n)} = (-1)^n (-x)_n \tag{7}$$

where $(x)^{(n)} = x(x+1)(x+2)\ldots(x+n-1)$ (cf. [1]-[22]).

The Apostol-Bernoulli polynomials, $\mathcal{B}_k(x,t)$ defined by Apostol [1]. These polynomials are given by means of the following generating function:

$$\frac{ze^{zx}}{te^z - 1} = \sum_{k=0}^{\infty} \mathcal{B}_k(x,t) \frac{z^k}{k!}, \tag{8}$$

where $|z| < 2\pi$ when $t = 1$ and $|z| < \left|\log t\right|$ when $t \neq 1$ and $t \in \mathbb{C}$. From the above generating function, we have $\mathcal{B}_m(t) = \mathcal{B}_m(0,t)$ denotes the Apostol-Bernoulli numbers. A recurrence relation for these numbers is given as follows:

$$\mathcal{B}_0(t) = 0, \mathcal{B}_1(t) = \frac{1}{t-1}, \mathcal{B}_m(t) = \frac{t}{1-t} \sum_{j=0}^{m-1} \left(\begin{array}{c} m \\ j \end{array} \right) \mathcal{B}_j(t). \tag{9}$$

Few values of the Apostol-Bernoulli numbers are given as follows:

$$\mathcal{B}_2(t) = \frac{-2t}{(t-1)^2}, \mathcal{B}_3(t) = \frac{3t(t+1)}{(t-1)^3}, \mathcal{B}_4(t) = \frac{-4t\left(t^2+4t+1\right)}{(t-1)^4},$$

$$\mathcal{B}_5(t) = \frac{5t\left(t^3+11t^2+11t+1\right)}{(t-1)^5}, \mathcal{B}_6(t) = \frac{-6t\left(t^4+26t^3+66t^2+26t+1\right)}{(t-1)^6},$$

(*cf.* [1], [4], [6], [16], [20], [21], [22]; and the references cited therein).

Explicit formula for the Apostol-Bernoulli numbers as follows:

$$\mathcal{B}_{m+1}(t) = \frac{m+1}{t-1} \sum_{n=0}^{m} \sum_{k=0}^{n} (-1)^k \left(\begin{array}{c} n \\ k \end{array} \right) \left(\frac{t}{t-1} \right)^n k^m \tag{10}$$

where $m \in \mathbb{N}_0$(*cf* [19]).

Remark 1.5. *Different proofs of the above formula are also given by Apostol [1] and Boyadzhiev [4].*

The Stirling numbers of the second kind $S(n,v)$ are defined by means of the following generating functions:

$$\sum_{v=0}^{n} S(n,v)(x)_v = x^n \quad \text{and} \quad \sum_{n=v}^{\infty} S(n,v) \frac{x^n}{n!} = \frac{1}{v!}(e^x - 1)^v. \tag{11}$$

We also have $S(0,0) = 1$, $S(n,v) = 0$ if $v > n$; $S(n,0) = 0$ if $n > 0$ and

$$S(n,v) = \frac{1}{v!}\sum_{j=0}^{v}\binom{v}{j}(-1)^j (v-j)^n \tag{12}$$

(*cf.* [7], [22]; and the references cited therein).

The explicit formula for computing the Apostol-Bernoulli numbers with the help of the Stirling numbers of the second kind as follows (*cf.* [1, p. 166, Eq-(3.7)]):

$$\mathcal{B}_n(t) = \frac{n}{t-1}\sum_{k=0}^{n-1} k!\left(\frac{t}{1-t}\right)^k S(n-1,k). \tag{13}$$

The above relation is also given by Boyadziev in [4].

We summarize our paper as follows: in Section 2, by modifying the generating functions $f_{L_B}(t,p)$, we give an explicit formula for these functions. In Section 3, we prove Theorem 1.3 and Theorem 1.4 for the higher-order derivative formulas for the generating functions $f_{L_B}(t,p)$. By using these formulas, we derive some novel identities including the Stirling numbers of the second kind, the Apostol-Bernoulli numbers and combinatorial sums related to binomial coefficients. By using derivative formulas, we derive some applications related to the k-ary Lyndon words and combinatorial sums. In Section 4, we give not only an algorithm for computing numerical values of higher-order derivative formulas for the generating functions $f_{L_B}(t,p)$, but also some numerical computations.

2. Modification of the generating functions $f_{L_B}(t,p)$

So far, there are many kind of generating function for the k-ary Lyndon words in the literature (see [11], [17]). Generating function methods and combinatorial sums provide tools to find new identites and relations on afromentioned numbers and polynomials. For instance, in [21], Srivastava studied combinatorial sums related to the Bernoulli, Euler and Genocchi polynomials by using their generating functions and in [18], Simsek studied on generating functions for the special polynomials. Therefore, we here improve and modify generating functions for the k-ary Lyndon words by the following theorem:

Theorem 2.1.

$$f_{L_B}(t,p) = -\frac{t}{p(t-1)^2} - \frac{1}{p}\sum_{n=0}^{p}\sum_{k=0}^{n}(-1)^k\binom{n}{k}\frac{t^n k^p}{(t-1)^{n+1}}. \tag{14}$$

Proof. Combining (10) with (4) and after some elementary calculation, we arrive at the desired result. □

Motivation of this theorem is to directly evaluate the value of $f_{L_B}(t,p)$ without using any special numbers or polynomials unlike the other generating functions for the Lyndon words in the literature and also in equation (4).

By using (14), we compute two values of the numbers $f_{L_B}(t,p)$ for $p = 2$ and $p = 3$ as follows:

$$f_{L_B}(t,2) = \frac{t^2}{(1-t)^3} \text{ and } f_{L_B}(t,3) = \frac{2t^2}{(t-1)^4}.$$

For other computation methods, see also the references [10] and [11].

We also substitute $t = \frac{1}{2}$, $p = 2$ and $p = 3$ into (14), we obtain

$$f_{L_B}\left(\frac{1}{2},2\right) = 2 \text{ and } f_{L_B}\left(\frac{1}{2},3\right) = 8.$$

By using (7) and negative binomial series expansion in (14), we give a hypergeometric representation of the generating function $f_{L_B}(t,p)$ by the following theorem:

Theorem 2.2.

$$f_{L_B}(t,p) = -\frac{t}{p(t-1)^2} - \frac{1}{p}\sum_{n=0}^{p}\sum_{k=0}^{n}(-1)^{n+k+1}\binom{n}{k}t^n k^p \, {}_1F_0\left(-n-1;-;-t\right)$$

where ${}_1F_0$ *denotes the hypergeometric functions given as follows:*

$${}_1F_0\left(-n-1;-;-t\right) = \sum_{m=0}^{\infty}(-n-1)_m\frac{(-t)^m}{m!}.$$

3. Derivative equations for the generating functions $f_{L_B}(t,p)$ and their numerical applications

The purpose of this section is to prove Theorem 1.3 and Theorem 1.4. By using these theorems, we give some identities relations associated with the Stirling numbers of the second kind, the Apostol-Bernoulli numbers and combinatorial sums. We also derive a formula for the higher-order derivative of $\mathcal{B}_p(t)$ at $t = 0$. Finally, some applications for these theorems are given.

In order to prove Theorem 1.3 and Theorem 1.4, we need the following lemma:

Lemma 3.1.

$$\frac{d^v}{dt^v}\{\mathcal{B}_2(t)\} = \frac{d^v}{dt^v}\left\{\frac{-2t}{(t-1)^2}\right\} = \frac{2(-1)^{v+1}v!(t+v)}{(t-1)^{v+2}}.$$

Proof. The proof of this lemma related to the operator $\frac{d^v}{dt^v}$. So, we omit it. □

3.1. Proof of Theorems

Proof. [Proof of Theorem 1.3] Substituting (13) into (4), we get

$$f_{L_B}(t,p) = -\frac{1}{p}\left(\frac{t}{(t-1)^2} + \frac{1}{t-1}\sum_{k=0}^{p}k!\left(\frac{t}{1-t}\right)^k S(p,k)\right).$$

Differentiating both side of the above equation with respect to t, we get the following derivative equations:

$$\frac{d}{dt}\{f_{L_B}(t,p)\} = -\frac{1}{p}\left[\frac{-(t+1)}{(t-1)^3} + \sum_{k=0}^{p}k!S(p,k)\left\{-\frac{1}{(t-1)^2}\left(\frac{t}{1-t}\right)^k + \frac{k}{(t-1)^3}\left(\frac{t}{1-t}\right)^{k-1}\right\}\right].$$

By iterating the above derivation for the variable t with the help of Lemma 3.1 and using induction method, we arrive at the assertation of Theorem 1.3. □

Proof. [Proof of Theorem 1.4] By using equation (9), we modify (4) as follows:

$$f_{L_B}(t,p) = -\frac{1}{p}\left(\frac{t}{(t-1)^2} - \frac{t}{(p+1)(t-1)}\sum_{j=0}^{p}\binom{p+1}{j}\mathcal{B}_j(t)\right).$$

Differentiating the above equation with respect to t, we get the following derivative equations:

$$\frac{d}{dt}\{f_{L_B}(t,p)\} = -\frac{1}{p}\left[\frac{-(t+1)}{(t-1)^3} - \frac{1}{p+1}\sum_{j=0}^{p}\binom{p+1}{j}\left\{-\frac{1}{(t-1)^2}\mathcal{B}_j(t) + \frac{t}{t-1}\frac{d}{dt}\{\mathcal{B}_j(t)\}\right\}\right].$$

By iterating the above derivation for the variable t with the help of Lemma 3.1 and using induction method, we arrive at the assertation of Theorem 1.4. □

3.2. Applications related to the derivative formulas

In this section, by using the derivative formulas, we give some applications.

By substituting $t = 0$ into equation (5), we get combinatorial sums for higher-order derivative of the generating functions for the numbers $L_k(n)$ by the following corollary:

Corollary 3.2.

$$\frac{d^v}{dt^v}\left\{f_{L_B}(t,p)\right\}\Big|_{t=0} = \frac{v!}{p}\left[-v + \sum_{j=0}^{v} j!\binom{v}{j} S(p,j)\right]. \tag{15}$$

By substituting $t = 0$ into equation (6), we get combinatorial sums for higher-order derivative of the generating functions for the numbers $L_k(n)$ by the following corollary:

Corollary 3.3.

$$\frac{d^v}{dt^v}\left\{f_{L_B}(t,p)\right\}\Big|_{t=0} = -\frac{1}{p}\left[v!v + \frac{1}{(p+1)}\sum_{j=0}^{p}\binom{p+1}{j}\sum_{k=0}^{v-1}\frac{v!}{k!}\frac{d^k}{dt^k}\{\mathcal{B}_j(t)\}\right]\Bigg|_{t=0}. \tag{16}$$

By using the above results, we give a novel combinatorial sums associated with the Stirling numbers of the second kind and the higher-order derivative of the Apostol-Bernoulli numbers.

Theorem 3.4.

$$\frac{1}{(p+1)}\sum_{j=0}^{p}\binom{p+1}{j}\left\{t\frac{d^v}{dt^v}\{\mathcal{B}_j(t)\} + \sum_{k=0}^{v-1}(-1)^{v-k}\frac{v!}{k!(t-1)^{v-k}}\frac{d^k}{dt^k}\{\mathcal{B}_j(t)\}\right\}$$
$$= -\frac{v!(-1)^v}{(t-1)^v}\sum_{k=0}^{p} k!S(p,k)\left\{\sum_{j=0}^{v}(-1)^j\binom{v}{j}\binom{k}{j}\frac{1}{(t-1)^j}\left(\frac{t}{1-t}\right)^{k-j}\right\}.$$

Proof. Proof of this theorem follows immediately from combining (5) and (6). □

Combining (15) and (16), we get the following differential equation including Apostol-Bernoulli numbers, with respect to t parameter, by the following theorem:

Theorem 3.5.

$$\left[\sum_{j=0}^{p}\sum_{k=0}^{v-1}\binom{p+1}{j}\frac{v!}{k!}\frac{d^k}{dt^k}\{\mathcal{B}_j(t)\}\right]\Bigg|_{t=0} = -v(p+1)\sum_{j=0}^{v} j!\binom{v}{j}S(p,j).$$

Remark 3.6. *Proof of the Theorem 3.5 is also obtained by Theorem 3.4 when $t = 0$.*

Corollary 3.7.

$$t(t-1)\sum_{j=0}^{p}\binom{p+1}{j}\frac{d}{dt}\{\mathcal{B}_j(t)\} = (p+1)\sum_{k=0}^{p} k!S(p,k)\frac{t+k}{t}\left(\frac{t}{1-t}\right)^k + \frac{1-t}{t}\mathcal{B}_{p+1}(t).$$

Proof. Substituting $v = 1$ into Theorem 3.4 and combining with equation (9), we arrive at the desired result. □

4. Computation algorithm

In this section, by combining explicit formula for the Stirling numbers of the second kind given by equation (12) with derivative formula in Theorem 1.3, we present an algorithm for computing numerical values of the higher-order derivative of the generating functions enumerating k-ary Lyndon words with prime number length.

Algorithm 1 Let p be a prime number, $v \in \mathbb{N}_0$ and $t \in \mathbb{C} \setminus \{1\}$. This algorithm will return the higher-order derivative of the generating functions for the numbers of the k-ary Lyndon words of prime number length p in (5) related to the Stirling numbers of the second kind(indicated by Stirling_Num_Second procedure).

```
procedure DERIVATIVE_GEN_FUNC_LYNDON(v: nonnegative integer, t, p: prime numbers)
    Begin
    Local variables: j ← 0, k ← 0, S ← 0
    for all k in {0, 1, 2, . . . , p} do
        for all j in {0, 1, 2, . . . , v} do
            S ← S + Power (−1, j) ∗ Binomial_Coef (v, j)
                ↪ ∗Binomial_Coef (k, j) ∗ Factorial (k)
                ↪ ∗Stirling_Num_Second (p, k) ∗ (1/Power (t − 1, j))
                ↪ ∗Power (t/ (1 − t) , k − j)
        end for
    end for
    return − (1/p) ∗ ((Power (−1, v) ∗ Factorial (v)) /Power (t − 1, v + 1))
                ↪ ∗ ((t + v) / (t − 1) + S)
end procedure
```

By applying this algorithm, we provide some numerical values of the first derivative of the functions $f_{L_B}(t,p)$ in the next section.

4.1. *Numerical computations for the first derivative of the functions $f_{L_B}(t,p)$ by the computation algorithm*

Here, by using the Algorithm 1, we present some numerical computations for the first derivative of the functions $f_{L_B}(t,p)$ on the first four prime numbers $p = 2; 3; 5; 7$ and $t = \frac{1}{2}$ as follows:

$$\frac{d}{dt}\{f_{L_B}(t,2)\}\Big|_{t=\frac{1}{2}} = 20, \qquad \frac{d}{dt}\{f_{L_B}(t,3)\}\Big|_{t=\frac{1}{2}} = 96,$$

$$\frac{d}{dt}\{f_{L_B}(t,5)\}\Big|_{t=\frac{1}{2}} = 3744, \qquad \frac{d}{dt}\{f_{L_B}(t,7)\}\Big|_{t=\frac{1}{2}} = 311904.$$

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