Combinatorics of poly-Bernoulli numbers

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Abstract: The $B_n^{(k)}$ poly-Bernoulli numbers — a natural generalization of classical Bernoulli numbers ($B_n = B_n^{(1)}$) — were introduced by Kaneko in 1997. When the parameter $k$ is negative then $B_n^{(-k)}$ is a natural number. Brewbaker was the first to give combinatorial interpretation of these numbers. He proved that $B_n^{(-k)}$ counts the, so called, lonesum 0-1 matrices of size $n \times k$. Several other interpretations were pointed out. We survey these and give new ones. Our new interpretation, for example, gives a transparent, combinatorial explanation of Kaneko’s recursive formula for poly-Bernoulli numbers.

Keywords: Poly-Bernoulli numbers, enumeration, combinatorial methods, bijective proofs, excluded submatrices

1 Introduction

In the 17th century Faulhaber [8] listed the formulas giving the sum of the $k^{\text{th}}$ powers of the first $n$ positive integers when $k \leq 17$. These formulas are always polynomials. Jacob Bernoulli [3] realized the scheme in the coefficients of these polynomials. Describing the coefficients he introduced a new sequence of rational numbers. Later Euler [7] recognized the significance of this sequence (that was connected his several celebrated results). He named the elements of the sequence as Bernoulli numbers. For example Bernoulli numbers appear in the closed formula for $\zeta(2k)$ (determining $\zeta(2)$ is the famous Basel problem, that was solved by Euler).

In 1997 Kaneko considered multiple zeta values (or Euler-Zagier sums). During his investigation he introduced the poly-Bernoulli numbers.

Definition 1 ([13]) The $\{B_n^{(k)}\}_{n \in \mathbb{N}, k \in \mathbb{Z}}$ poly-Bernoulli numbers are defined by the following exponential generating function

$$\sum_{n=0}^{\infty} B_n^{(k)} \frac{x^n}{n!} = \frac{Li_k(1-e^{-x})}{1-e^{-x}}, \quad \text{for all } k \in \mathbb{Z}$$

where

$$Li_k(x) = \sum_{i=1}^{\infty} \frac{x^i}{i^k}.$$ 

The sequence $\{B_n^{(1)}\}_n$ is just the classical (second) Bernoulli numbers. Later Kaneko gave a recursive definition of the poly-Bernoulli numbers:

Theorem 2 ([14], quoted in [10])

$$B_n^{(k)} = \frac{1}{n+1} \left( B_n^{(k-1)} - \sum_{m=1}^{n-1} \binom{n}{m-1} B_m^{(k)} \right).$$

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or equivalently

\[ B_n^{(k-1)} = B_n^{(k)} + \sum_{m=1}^{n} \binom{n}{m} B_{n-(m-1)}^{(k)}. \]

We need a more combinatorial description of poly-Bernoulli numbers, given by Arakawa and Kaneko.

**Definition 3** Let \( a \) and \( b \) be two natural numbers. A Stirling numbers of the second kind is the number of partitions of \([a] := \{1, 2, \ldots, a\}\) (or any set of \( a \) elements) into \( b \) classes, and is denoted by \( \{\binom{a}{b}\}\).

Partitions can be described as equivalence relations ([9]).

**Theorem 4** ([1]) For any natural numbers \( n \) and \( k \) the following formula holds

\[ B_n^{(-k)} = \sum_{m=0}^{n} m! \binom{n+1}{m+1} m! \binom{k+1}{m+1}. \]

This theorem exhibits the fact that \( B_n^{(-k)} \) numbers are natural numbers. This formula has initiated the combinatorial investigations of poly-Bernoulli numbers. There are several combinatorially described sequence of sets, such that their size is \( B_n^{(-k)} \) (we call them poly-Bernoulli families). We can consider these statements as alternative definitions of poly-Bernoulli numbers as answers to enumeration problems.

These combinatorial definitions give us the possibility to explain previous identities — originally proven by algebraic methods — combinatorially.

The importance of the notion of poly-Bernoulli numbers is underlined by the fact that there are several drastically different combinatorial descriptions.

After reviewing the previous works we give a new poly-Bernoulli family. In our family we consider 0-1 matrices with certain forbidden submatrix. So our enumerated matrices of size \( n \times k \) contain at most linear number of 1’s (at most \( n + k - 1 \)). Among Brewbaker’s lonesum matrices (in contrast) there are ones with many 1’s and there are others with few 1’s. We do not know direct bijection between lonesum matrices and matrices with no \( \Gamma \) (see section 3). Our main result is a bijective ([20], [21]) proof that matrices of size \( n \times k \) with no \( \Gamma \) is given by the formula in Theorem 4.

Finally some classical results are explained combinatorially.

The most recent research on poly-Bernoulli numbers is mostly number theoretical, analytical investigations and extensions ([2], [12], [18]). The combinatorial approach is different, but it might shed light on some connections and might lead to new directions.

# 2 Previous poly-Bernoulli families

## 2.1 The obvious interpretation

Seeing the formula of Arakawa and Kaneko one can easily come up with a combinatorial problem such that the answer to it is \( B_n^{(-k)} \).

Let \( N \) be a set of \( n \) elements and \( K \) a set of \( k \) elements. One can think as \( N = \{1, 2, \ldots, n\} =: [n] \) and \( K = [k] \). Extend both sets with a special element: \( \hat{N} = N \cup \{n+1\} \) and \( \hat{K} = K \cup \{k+1\} \). Take \( \mathcal{P}_{\hat{N}} \) a partition of \( \hat{N} \) and \( \mathcal{P}_{\hat{K}} \) a partition of \( \hat{K} \) with the same number of classes as \( \mathcal{P}_{\hat{N}} \). Both partitions have a special class: the class of the special element. We call the other classes as ordinary classes. Let \( m \) denote the number of ordinary classes in \( \mathcal{P}_{\hat{N}} \) (that is the same as the number of ordinary classes in \( \mathcal{P}_{\hat{K}} \)). Obviously \( m \in \{0, 1, 2, \ldots, \min\{n, k\}\} \). Order the ordinary classes arbitrarily in both partitions. How many ways can we do this?

For fixed \( m \) choosing \( \mathcal{P}_{\hat{N}} \) and ordering its ordinary classes can be done \( m! \binom{n+1}{m+1} \) ways. Choosing the pair of ordered partitions can be done \( m! \binom{k+1}{m+1} \) ways. The answer to our question is

\[ \sum_{m=0}^{n} m! \binom{n+1}{m+1} m! \binom{k+1}{m+1} = B_n^{(-k)}. \]
2.2 Lonesum matrices

Definition 5 A 0-1 matrix is lonesum iff it can be reconstructed from its row and column sums.

Obviously a lonesum matrix cannot contain the
\[
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}, \quad \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\]
submatrices (a submatrix is a matrix that can be obtained by deletion of rows and columns). Indeed, in the case of the existence of one of the forbidden submatrices we can switch it to the other one. This way we obtain a different matrix with the same row and column sums. It turns out that this property is a characterization [17].

It is obvious that in a lonesum matrix for two rows ‘having the same row sum’ is the same relation as ‘being equal’. Even more for rows \(r_1\) and \(r_2\) ‘the row sum in \(r_1\) is at least the row sum in \(r_2\)’ is the same as ‘\(r_1\) has 1’s in the positions of the 1’s of \(r_2\)’. The same is true for columns. An other easy observation is that changing the order of the rows/columns does not affects the lonesum property. These two observations guarantee that a lonesum matrix can be rearranged by row/column order changes into a matrix where the 1’s occupy positions such that they form a Young diagram ([9]). This is also a characterization of lonesum matrices.

¿From this new characterization one can see that the number of different non-0 row sums is the same as the number of different non-0 column sums.

Let \(M\) be a 0-1 lonesum matrix of size \(n \times k\). Add a special row and column with all 0’s. Let \(\tilde{M}\) be the extended \((n + 1) \times (k + 1)\) matrix. ‘Having the same row sum’ is an equivalence relation. The corresponding partition has a special class, the set of 0 rows. By the extension we ensured that the special class exists/non-empty. Let \(m\) be the number of non-special/ordinary classes. The ordinary classes are ordered by their corresponding row sums. The same way we obtain an ordered partition of columns. Straight forward to prove that the two ordered partitions give a coding of lonesum matrices. this gives us the following theorem of Brewbaker, first presented in his MSc thesis.

**Theorem 6 ([4],[5])** Let \(L_n^{(k)}\) the set of lonesum 0-1 matrices of size \(n \times k\). Then
\[
|L_n^{(k)}| = \sum_{m=0}^{n-k} \frac{m!}{m!} \binom{n+k-1}{k+1} = B_n^{(-k)}.
\]

2.3 Callan permutations and ascending-to-max permutations

Callan [6] considered the set \([n+k]\). We call the elements 1, 2, \ldots, \(n\) left-value elements (\(n\) many of them) and \(n+1, n+2, \ldots, n+k\) right-value elements (\(k\)-many of them). We extend our universe with 0, a special left-value element and with \(n+k+1\), a special right-value element. Let \(N = [n]\), \(K = \{n+1, n+2, \ldots, n+k\}\), \(\tilde{N} = [0] \cup [n]\), \(\tilde{K} = K \cup \{n+k+1\}\). Consider
\[
\pi : 0, \pi_1, \pi_2, \ldots, \pi_{n+k}, n + k + 1
\]
a permutation of \(\tilde{N} \cup \tilde{K}\) with the restriction that its first element is 0 and its last element is \(n + k + 1\). Consider the following equivalence relation/partition of left-values: two left-values are equivalent if ‘each element in the permutation between them is a left-value’. Similarly one can define an equivalence relation on the right-values: ‘each element in the permutation between them is a right-value’. The equivalence classes are just the “blocks” of left- and right-values in permutation \(\pi\). The left-right reading of \(\pi\) gives an ordering of left-value and right-value blocks/classes. The order starts with a left-value block (the equivalence class of 0, the special class) and ends with a right-value block (the equivalence class of \(n + k + 1\), the special class). Let \(m\) be the common number of ordinary left-value blocks and ordinary right-value blocks.
Callan considered the permutation such that in each block the numbers are in increasing order. Let \( C^{(k)}_n \) the set of these permutations. For example
\[
C^{(2)}_2 = \{012345, 013245, 014235, 013425, 023145, 024135, 023415, 031245, 031425, 032415, 034125, 041235, 041325, 042315, 042315\}
\]
(the right-value numbers are in boldface).

It is easy to see that describing a Callan permutation we need to give the two ordered partitions of the left-value and right-value elements. Indeed, inside the blocks the ‘increasing’ condition defines the order, and the ordering of the classes let us know how to merge the left-value and right-value blocks. We obtained the following theorem.

**Theorem 7**
\[
|C^{(k)}_n| = \sum_{m=0} m! \binom{n + 1}{m + 1} m! \binom{k + 1}{m + 1} = B^{(k)}_n.
\]

He, Munro and Rao [11] introduced the notion of max-ascending-permutations. This is (in some sense) a “dual” of the notion of Callan permutation. We mention that [19] does not contain this description of poly-Bernoulli numbers. Now we give a slightly different version of max-ascending-permutations that the one presented in [11].

Again we consider
\[
\pi : 0, \pi_1, \pi_2, \ldots, \pi_{n+k}, n + k + 1
\]
permutations of \( \hat{N} \cup \hat{K} \) with the restriction that its first element is 0 and its last element is \( n + k + 1 \). We call the first \( k + 1 \) elements of the permutation left-position elements (0 will be referred to as special left-position element). Consider the following equivalence relation/partition of left-positions: two left-positions are equivalent iff ‘each value between the ones, that occupy the positions, is in a left-position’. Similarly one can define an equivalence relation on the right-positions: ‘each value between the ones, that occupy the positions, is in a right-position’. The max-ascending-permutations property is that in a class of positions our numbers must be in increasing order.

The duality is a position-value exchanging duality. The following theorem is obvious from the discussion.

**Theorem 8** Let \( A^{(k)}_n \) the set of max-ascending-permutations of \( \{0, 1, 2, \ldots, n + k + 1\} \). Then
\[
|A^{(k)}_n| = \sum_{m=0} m! \binom{n + 1}{m + 1} m! \binom{k + 1}{m + 1} = B^{(k)}_n.
\]

We give an example
\[
A^{(2)}_2 = \{012345, 012345, 013245, 031245, 014235, 014235, 023145, 031245, 024135, 024135, 024315, 042135, 042315, 042315\},
\]
where boldface denotes the numbers at right-positions.

### 2.4 Vesztergombi permutations

Vesztergombi [22] investigated permutations of \( [n + k] \) with the property that \(-k < \pi(i) - i < n\). She determined a formula for their number. Lovász [16] give a combinatorial presentation of this result. Launois working on quantum matrices slightly modified Vesztergombi’s set and realized the connection to poly-Bernoulli numbers. The significant part of this line of research is summarized in the following theorem.

**Theorem 9** Let \( V^{(k)}_n \) the set of permutations \( \pi \) of \( [n + k] \) such that \(-k \leq \pi(i) - i \leq n\) for all \( i \) in \( [n + k] \).
\[
|V^{(k)}_n| = \sum_{m=0} m! \binom{n + 1}{m + 1} m! \binom{k + 1}{m + 1} = B^{(k)}_n.
\]
3 A new poly-Bernoulli family

Let $M$ be a 0-1 matrix. We say that three 1’s in $M$ form a $\Gamma$ configuration iff they are the NE, NW and SW elements of a a submatrix of size $2 \times 2$. So we do not have any condition on the SE element of the submatrix of size $2 \times 2$, containing the $\Gamma$.

We will consider matrices without $\Gamma$ configuration. Let $G_n^{(k)}$ the set of all 0-1 matrices without $\Gamma$.

The following theorem is our main theorem.

**Theorem 10**

$$|G_n^{(k)}| = B_n^{(-k)}.$$  

The rest of the section is devoted to the combinatorial proof of this statement. The obvious way to prove our claim is to give a bijection to one of the previous sets, where the size is known to be $B_n^{(-k)}$. The obvious candidate is $L_n^{(k)}$. We do not know straight, simple bijection between these two sets of matrices.

Instead, we follow the obvious scheme: we code $\Gamma$-free matrices with two partitions and two orders. From this and from the previous bijections one can construct a direct bijection between the two sets of matrices but that is not appealing.

Let $M$ be a 0-1 matrix of size $n \times k$. We say that a position/element has height $n-i$ iff it is in the $i$th row. The top-1 of a column is its 1 element of maximal height. The height of the column is the height of its maximal 1 or 0, whenever it is a 0 column.

Let $M$ be a matrix without $\Gamma$ configuration. Let $\tilde{M}$ be the extension of it with an all 0’s column and row. ‘Having the same height’ is an equivalence relation on the set of columns in $\tilde{M}$. The class of the special column is the set of 0 columns (that is not empty since we work with the extended matrix). Let $m$ be the number of the non-special classes. These $m$ classes partition the set of non-0 columns. Take $\mathcal{C}$, any non-special class of columns (the columns in $\mathcal{C}$ is ordered as the indices order the whole set of columns). Since our matrix does not contain $\Gamma$ all columns but the last one has only one 1 (that is necessarily the top-1) of the same height. We say that the last elements/columns of non-special classes are **important columns**. Important columns in $\tilde{M}$ form a submatrix $M_0$ of size $(n+1) \times m$. In $M_0$ the top-1’s are called **important elements**. In each row without top-1 the leading 1 (the 1 with minimal column index) is also called **important 1**. So in all non-0 rows of $M_0$ there is exactly one important 1. ‘Our important 1s are in the same columns’ is an equivalence relation on the set of rows in $M_0$ (where the zero rows form a special class). The top-1’s guarantee that we have $m$ many non-special row classes. In any non-special class there is one top-1. This way the top-1’s establish a bijection between the $m$ non-special classes of columns and non-special classes or rows.

A partition of columns into $m+1$ classes, and partition of rows into $m+1$ classes, and a bijection between the non-special row- and column-classes — after fixing $m$ — leaves

$$m! \left\{ \begin{array}{c} n+1 \\ m+1 \end{array} \right\} \left\{ \begin{array}{c} k+1 \\ m+1 \end{array} \right\}$$

possibilities. This information (knowing the two partitions and the correspondence) codes a big part of matrix $\tilde{M}$:

We know that the columns and rows of the special-classes are all 0’s. A non-special column class $\mathcal{C}$ has a corresponding class of rows. The top row of the corresponding row class gives us the common height of the columns in $\mathcal{C}$. So we know each non-important columns (they have only one 1, defining its known height). We narrowed the unknown 1’s of $M$ into the non-0 rows of $M_0$. Easy to check that $\tilde{M}$ contains $\Gamma$ iff $M_0$ contains one.

Now on we concentrate on $M_0$. The position of important ones can be reconstructed easily. In each column of $M_0$ there is a lowest important 1. We call them **crucial 1’s**. (Specially crucial 1’s are important 1’s too.) A 1 in $M_0$ that is non-important is called **hiding 1**.

**Lemma 11** Consider a hiding 1 in $M_0$. Then exactly one of the following two possibilities holds:
(1) there is a crucial 1 above it and a top-1 to the right of it,
(2) there is a crucial 1 on its left side (and of course a top-1 above it).

Proof: Let \( h \) be a hiding 1 in \( M_0 \).

First, assume that the row of \( h \) does not contain a top-1. Then the first 1 in this row \( (f) \) is an important 1 (hence it differs from \( h \)). Since the matrix is \( \Gamma \)-free, we cannot have a 1 under \( f \), i.e. \( f \) is a crucial 1. \( h \) is not important, so it is not a top-1. The top-1 in its column must be above it. We obtained that case (2) holds.

Second, assume that the row of \( h \) contains a top-1, \( t \). If \( t \) is on the left of \( h \) then the forbidden \( \Gamma \) ensures that under \( t \) there is no other 1. Hence \( h \) is crucial and case (2) holds again. If \( t \) is on the right of \( h \) then the forbidden \( \Gamma \) ensures that under \( h \) there is no other 1. Hence the lowest important 1 in the column of \( h \) (a crucial 1) is above of it. Case (1) holds.

(1) and (2) cases are exclusive since if both are satisfied then \( h \) has a crucial 1 on its left and a top-1 on its right. That is impossible since the 1’s in a row of a top-1 are not even important.

Take a crucial 1 in \( M_0 \), that we call \( c \). For any top-1, \( t \) that comes in a later column and it is higher than \( c \) the position in the row of \( c \) under \( t \) we call questionable. Also for any top-1, \( t \) that comes in a later column and it is lower than \( c \) the position in the column of \( c \) before \( t \) we call questionable.

The meaning of the lemma is that each hiding 1 is in a questionable position. Moreover each questionable position has a corresponding crucial 1. We say that the corresponding crucial 1 is responsible for that questionable position. Let \( c \) be a crucial 1. Assume that there are \( i \) many columns following \( c \)’s column in \( M_0 \). Then there are \( i \) questionable position such that \( c \) is responsible for that.

The following picture gives an example with a crucial 1 \( (1^{(c)}) \), with four following columns and with four ?’s denoting the positions of the four questionable positions. The top-1’s of the four columns are circled. The arrows are just helping the reader to identify the corresponding top-1.

\[
\begin{pmatrix}
... \\
... \\
... \\
... \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
1^{(c)} \\
? \\
? \\
? \\
? \\
... \\
\end{pmatrix}
\]

It is obvious that we have \((m - 1) + (m - 2) + \ldots + 2 + 1\) many questionable positions.

Corollary 12 All hiding 1’s are in questionable positions.

Easy to check that if we put the important 1’s into \( M_0 \) and add a new 1 into a questionable position then we won’t create a \( \Gamma \) configuration. The problem is that the different questionable positions are not independent.

Lemma 13 There are \( m! \) ways to fill the questionable positions with 0’s and 1’s without forming a \( \Gamma \).

The lemma finishes the enumeration of \( \Gamma \)-free 0-1 matrices of size \( n \times k \). Also finishes a description of a constructive bijection from \( M_{n}^{(k)} \) to the obvious poly-Bernoulli set. Our main theorem is proven.
4 Combinatorial proofs

Theorem 14

\[ B_n^{(-k)} = B_k^{(-n)}. \]

The relation originally was proven by Kaneko. It is obvious from any of the combinatorial definitions. Arakawa–Kaneko formula also exhibits this symmetry an algebraic way.

Theorem 15

\[ B_n^{(-k)} = B_n^{(-(k-1))} + \sum_{i=1}^{n} B_{n-i}^{(-k-1)}. \]

Proof: Our main theorem gives that \( B_n^{(-k)} \) counts the \( \Gamma \)-free matrices of size \( n \times k \). Partition \( M_n^{(k)} \) according to the number of 1’s in its first column. Let us denote this number by \( i \).

If \( i = 0 \) (i.e. the first column is an all 0’s column), then we need to choose the rest of the matrix freely, that is \( B_k^{(-n)} \) possibilities. If \( i > 0 \), then the \( \Gamma \)-free property ensures that the row of the \( i \) 1-s in the first column except the lowest one cannot contain any other 1. The rest \( n - (i-1) \) many rows can be filled \( B_{n-i}^{-(k-1)} \) many ways to avoid the \( \Gamma \) configuration.

The recursion is proven. \( \square \)

References


