Computations about formal multiple zeta spaces defined by binary extended double shuffle relations

Tomoya Machide∗

Abstract

The formal multiple zeta space we consider with a computer is an \( \mathbb{F}_2 \)-vector space generated by \( 2^k - 2 \) formal symbols for a given weight \( k \), where the symbols satisfy binary extended double shuffle relations. Up to weight \( k = 22 \), we compute the dimensions of the formal multiple zeta spaces, and verify the dimension conjecture on original extended double shuffle relations of real multiple zeta values. Our computations adopt Gaussian forward elimination and give information for spaces filtered by depth. We can observe that the dimensions of the depth-graded formal multiple zeta spaces have a Pascal triangle pattern expected by the Hoffman mult-indices.

1 Introduction

The space generated by multiple zeta values (MZVs for short) has been elucidated theoretically and numerically in recent years, but its structure remains mysterious. In this paper, we shed light on a formal space generated by binary analogs of MZVs by computer experiments for unraveling both of the original and formal spaces.

Let \( \mathbb{N} \) denote the set of positive integers. The MZV is a real number that belongs to an image of a function (customarily denoted by \( \zeta \)) whose domain is

\[
I = \bigcup_{r \geq 0} \{ k_r = (k_1, k_2, \ldots, k_r) \in \mathbb{N}^r \mid k_1 \geq 2 \},
\]

where \( k_0 = \emptyset \) is the empty mult-index and \( \zeta(\emptyset) = 1 \). We call \( w(k_r) = k_1 + \cdots + k_r \) and \( d(k_r) = r \) the weight and depth, respectively. The function \( \zeta \) has two definitions by the iterated integral and nested summation, which endow the \( \mathbb{Q} \)-vector space \( \mathcal{Z} \) spanned by MZVs with abundant linear relations. Euler [12], who solved the Basel problem \( \zeta(2) = \pi^2/6 \) and advanced the case \( r = 1 \), also studied the case \( r = 2 \).

Zagier [33] conjectured\(^1\) that \( \mathcal{Z} \) is graded by weight and the dimensions of graded pieces are expressed in terms of a Fibonacci-like sequence. Let \( I_k \) be the subset consisting of mult-indices of weight \( k \), and let \( \mathcal{Z}_k \) be the subspace spanned by MZVs in \( \zeta(I_k) = \{ \zeta(k) \mid k \in I_k \} \). The dimension conjecture is

\[
\dim_{\mathbb{Q}} \mathcal{Z}_k \overset{?}{=} d_k,
\]

where \( d_k = d_{k-2} + d_{k-3} \) (\( k \geq 3 \)), \( d_0 = d_2 = 1 \) and \( d_1 = 0 \). These integers fit together into the generating series

\[
\sum_{k \geq 0} d_k X^k = \frac{1}{1 - (X^2 + X^3)}.
\]

∗National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan
E-mail : machide@nii.ac.jp
MSC-class: 11M32 (Primary); 15A03,68W30 (Secondary)
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\(^1\)Zagier noted the conjectures were made after many discussions with Drinfel’d, Kontsevich and Goncharov.
The ultimate upper bound theorem (i.e., $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq d_k$) was established independently by Goncharov [9, 15] and Terasoma [31]. Brown [7] furthermore proved that $\mathcal{Z}_k$ is generated by MZVs in $\zeta(I_k^H)$, where $I_k^H$ is the set of Hoffman mult-indices of weight $k$:

$$I_k^H = \{\mathbf{k} = (k_1, \ldots, k_r) \in I_k \mid k_i \in \{2,3\}\}. \quad (1.4)$$

Hoffman [17] conjectured $\zeta(I_k^H)$ is a basis of $\mathcal{Z}_k$, which would imply the dimension conjecture because the same recurrence relation $|I_k^H| = |I_{k-2}^H| + |I_{k-3}^H|$ holds by a simple count of the number of 2’s and 3’s. Umezawa [32] also suggested a basis conjecture in terms of iterated log-sine integrals, in which sets of mult-indices different from $I_k^H$ are used. Because of the difficulty to show the independence between MZVs, no non-trivial lower bounds are known.

By the upper bound theorem, it is natural to ask that what sorts of relations are needed to reduce the number of generators of $\mathcal{Z}_k$ to $d_k$. There are several conjectural candidates: e.g., [10, 13, 16, 21, 22]. In particular, the extended double shuffle (EDS) relations [18, 28] known from early on are often selected for experimentally attacking this question, because they are easier to write down and included in the other candidates except Kawasima’s [22]. Minh and Petitot [27] verified that the class of EDS relations is a right candidate up to weight 10, Bigotte et al. [4] verified it up to weight 12, Minh et al. [26] verified it up to weight 16, Espie et al. [11] verified it up to weight 19, and Kaneko et al. [20] verified it up to weight 20 that seems to be the latest record. The first two experiments are by the Gröbner basis method, and the last three ones are by the vector space (or matrix) method. The fourth one of [11] was executed under modulo rational multiples of powers of $\zeta(2)$, or module $\mathbb{Q}[\zeta(2)]$.

The first purpose of this paper is to improve the record to weight $k = 22$. For this, we consider an $\mathbb{F}_2$-vector space $\mathcal{Z}_k^b$ instead of the $\mathbb{Q}$-vector space $\mathcal{Z}_k$: roughly speaking, $\mathcal{Z}_k^b$ is generated by binary multiple zeta symbols $\zeta^b(k)$ ($k \in I_k$) (binary MZSs for short), where $\zeta^b(k)$ satisfy binary EDS relations that are obtained from original EDS relations after the modulo 2 arithmetic to integer coefficients. (Exact definitions of the binary analogs in this section will be stated in the next section.) We will verify $\zeta^b(I_k^H) = \mathcal{Z}_k^b$ is a basis of $\mathcal{Z}_k^b$ and $\dim_{\mathbb{F}_2} \mathcal{Z}_k^b = d_k$. Our calculation results break the record because $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq \dim_{\mathbb{F}_2} \mathcal{Z}_k^b$ (as will be mentioned in Section 3). The space $\mathcal{Z}_k^b$ reduces the computation cost since $\mathbb{F}_2$ is the binary and simplest finite field. The field $\mathbb{F}_2$ makes it easy to apply useful techniques in computer since $\mathbb{F}_2$ is compatible with the Boolean data type: in fact, we will employ a conflict based algorithm discussed in [23] for a fast Gaussian forward elimination.

The second and main purpose is to observe a Pascal triangle pattern in $\mathcal{Z}_k^b$ from the viewpoint of a direct sum decomposition,

$$\mathcal{Z}_k^b \cong \mathcal{Z}_{k,0}^{b} \oplus \cdots \oplus \mathcal{Z}_{k,0}^{b}, \quad (1.5)$$

where $\mathcal{Z}_{k,r}^{b}$ are quotient spaces defined by means of depth filtration: the descending chain $\mathcal{Z}_{k-1}^{b} \supset \cdots \supset \mathcal{Z}_{k,0}^{b}$ is used for $\mathcal{Z}_{k,r}^b = \mathcal{Z}_{k,r}^b / \mathcal{Z}_{k,r-1}^b$, where $\mathcal{Z}_{k,r}^b$ are the subspaces spanned by binary MZSs of weight $k$ and depth at most $r$. We define $I_{k,r} = \{\mathbf{k} \in I_k \mid d(\mathbf{k}) = r\}$ and

$$I_{k,r}^H = I_k^H \cap I_{k,r}, \quad (1.6)$$

with $d_{k,r} = |I_{k,r}^H|$. We denote by $\zeta^b(k)$ the canonical image\(^3\) of $\zeta^b(k)$ in $\mathcal{Z}_{k,r}^b$ for any $k \in I_{k,r}$.

Up to weight $k = 22$, we will verify $\zeta^b(I_k^H)$ is a basis of $\mathcal{Z}_k^b$ and $\dim_{\mathbb{F}_2} \mathcal{Z}_{k,r}^b = d_{k,r}$. Counting the number of 2’s and 3’s implies that the double sequence $(d_{k,r})$ satisfies a recurrence relation

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\(^2\)This experimental result was announced in their private communication (see [20, Section 1]).

\(^3\)We use the same notation $\zeta^b(k)$ for all canonical images in the quotient spaces $\mathcal{Z}_{k,r}^b (k > r \geq 0)$. There should be no confusion because the quotient space under consideration is clear from context.
with a Pascal triangle pattern: $d^b_{k,r} = d^b_{k-2,r-1} + d^b_{k-3,r-1}$ ($k \geq 3, r \geq 1$), $d^b_{0,0} = d^b_{2,1} = 1$ and $d^b_{k,r} = 0$ for other $k$ and $r$, or equivalently,

$$
\sum_{k,r \geq 0} d^b_{k,r} X^k Y^r = \frac{1}{1 - (X^2 + X^3)Y}.
$$

(1.7)

More precisely, $d^b_{k,r} = \binom{k}{r}$ since the integers $P_{r,k} = d^b_{k+2r,r}$ satisfy the same recurrence relation as the binomial coefficients $\binom{k}{r}$. As expected from (1.5), the formula (1.7) specializes to (1.3) upon $Y = 1$.

We also try experiments on parts of EDS relations, ‘KNT’ and ‘MJPO’ relations, which are expected to be alternatives to EDS and actually employed in [20, 26] for verification, respectively. Unlike the case in $\mathbb{Z}_k$, those relations do not suffice to give all relations in $\mathbb{Z}^b_k$, but we can find a quasi Fibonacci-like rule in dimensions of spaces defined by MJPO relations.

The idea of the depth filtration in (1.5) was conceived by Broadhurst and Kreimer [6] to propose a refinement of the dimension conjecture. Their conjecture indicates two interesting facts in the $\mathbb{Q}$-vector spaces of MZVs graded by both weight and depth: (i) modular forms influence the structure through quotient spaces $\mathbb{Z}_{k,r}$ defined by the $\mathbb{Q}$-version of (1.5); and (ii) the Hoffman values $\zeta^b(k)$ ($k \in \mathbb{I}^H_k$) are irrelevant to the structure in the sense that most of the values vanish in the graded pieces of same depth. In terms of the generating series, the conjecture is

$$
\sum_{k,r \geq 0} \dim \mathbb{Z}_{k,r} X^k Y^r = \frac{1 + E(X)Y}{1 - O(X)Y + S(X)Y^2(1 - Y^2)},
$$

(1.8)

where $E(X) = X^2/(1 - X^2)$, $O(X) = X^3/(1 - X^2)$ and $S(X) = X^{12}/(1 - X^4)(1 - X^6)$, and $S(X)$ is the generating series of the dimensions of the vector spaces of cusp forms on the full modular group. Specific examples for $r = 2$ are given in [14] and a modern formulation is discussed in [8] (see also [30]). However our computational results suggest the following when we adopt $\mathbb{F}_2$ as the scalar field instead of $\mathbb{Q}$: (i) the influence of modular forms disappears; but (ii) the Hoffman symbols $\zeta^b(k)$ ($k \in \mathbb{I}^H_k$) remain as basis elements with a Pascal triangle pattern.

It should be noted that the Broadhurst-Kreimer conjecture has two equivalent formulations of vector and algebra (see [18, Appendix]). The equivalence requires $\mathbb{Q}[\zeta(2)]$ is isomorphic to the polynomial ring in one variable over $\mathbb{Q}$. The isomorphism does not hold when $\mathbb{F}_2$ is the scalar field as will be mentioned in the final section, and we will consider only the vector formulation in this paper.

It should also be noted that Blümlein et al. [5] provided a data mine for not only MZVs but also Euler sums by experiments to Broadhurst-Kreimer type conjectures, in which it was verified that the union of EDS and duality relations suffices to reduce the number of generators of $\mathbb{Z}_k$ to $d_k$ up to weight 22: it was also verified up to 24 by using modular arithmetic, and up to 26 and more with an additional conjecture and limited depths. The duality relations, which are obtained by the integral definition of MZVs and a change of variables, are very useful to compute because they can bring down the size of relations by about half. It has not been proved yet that the EDS relations include the duality relations, although the inclusion is expected to be true conjecturally: in other words, we have not succeeded in understanding the duality of MZVs algebraically. The experimental approaches of [5] and ours differ in the use of the duality relations.

The organization of this paper is as follows. In Section 2, we state exact definitions of the binary MZVs $\zeta^b(k)$, the formal multiple zeta spaces $\mathbb{Z}^b_k$ and the quotient spaces $\mathbb{Z}^b_{k,r}$. We report our computational results in Section 3, and explain how our computer programs
produce the results in Section 4. The programs are available at the open-source site GitHub.\textsuperscript{4} Section 5 is devoted to problems about formal multiple zeta spaces which arise from the computational results. In Appendix, we describe an essential algorithm in our experiments, which employs a conflict based search and speeds up the Gaussian forward elimination under certain conditions.

The computer only assists us in showing Proposition 4.1 by Gaussian elimination. The dimension conjecture (1.2) is true if we can theoretically show Proposition 4.1 for all weights \( k \).

2 Formal multiple zeta space over \( \mathbb{F}_2 \)

The formal multiple zeta space \( Z^b_k \) of weight \( k \) is briefly defined by

\[
Z^b_k = \frac{\{\eta^b(k) | k \in I_k \}}{\{\text{binary EDS relations}\}}, \tag{2.1}
\]

where \( \eta^b(k) \) are indeterminates. That is, \( Z^b_k \) is an \( \mathbb{F}_2 \)-vector space generated by formal symbols \( \zeta^b(k) \equiv \eta^b(k) \) that satisfy binary variations of the EDS relations. Eight equivalent statements are given in [18, Theorem 2] for the EDS relations. In this paper, we choose the statement (v) in the theorem because the relations are all \( \mathbb{Z} \)-linear and fewer in number.

To define (2.1) exactly, we require the algebraic setup by Hoffman [17] which allows us the steady handling of two products, the shuffle \( \shuffle \) and stuffle \( \ast \): the latter is also called harmonic or quasi-shuffle. Let \( \mathcal{H} \) be the polynomial ring \( \mathbb{Q}\langle x, y \rangle \) in the two non-commutative variables \( x \) and \( y \). We call each variable a letter, and a monomial in the variables a word. The shuffle product \( \shuffle \) is a \( \mathbb{Q} \)-bilinear product on \( \mathcal{H} \), which satisfies \( w = \shuffle \ 1 = 1 \shuffle w \) and

\[
a u \shuffle b v = a(u \shuffle b v) + b(a \shuffle u \shuffle v) \tag{2.2}
\]

for any words \( u, v, w \in \mathcal{H} \) and letters \( a, b \in \{ x, y \} \). Let \( z_k \) denote a word \( x^{k-1}y \) for any \( k \geq 1 \), and let \( \mathcal{H}^1 \) be the polynomial ring \( \mathbb{Q}\langle z_1, z_2, \ldots \rangle \), or equivalently, the subring \( \mathbb{Q} \oplus \mathcal{H}y \) in \( \mathcal{H} \). The shuffle product \( \ast \) is a \( \mathbb{Q} \)-bilinear product on \( \mathcal{H}^1 \), which satisfies \( w = \ast 1 = 1 \ast w \) and

\[
\begin{array}{l}
z_i u \ast z_j v = z_i (u \ast z_j v) + z_j (z_i u \ast v) + z_{i+j} (u \ast v) \tag{2.3}
\end{array}
\]

for any words \( u, v, w \in \mathcal{H} \) and integers \( i, j \geq 1 \). By induction on the lengths of words, both products are commutative and associative, and both \( \mathcal{H}^1_m = (\mathcal{H}^1, \shuffle) \) and \( \mathcal{H}^1 = (\mathcal{H}^1, \ast) \) are commutative \( \mathbb{Q} \)-algebras. We notice \( \mathcal{H}^1_m = (\mathcal{H}^1, \shuffle) \) is a parent space of \( \mathcal{H}^1_m \). Let \( \mathcal{H}^0 = \mathbb{Q} + xy \mathcal{H} = \langle z_k | k \in I \rangle_{\mathbb{Q}} \), where \( z_k = z_{k_1} \cdots z_{k_r} \) and \( z_0 = 1 \). Both \( \mathcal{H}^0_m = (\mathcal{H}^0, \shuffle) \) and \( \mathcal{H}^0 = (\mathcal{H}^0, \ast) \) are subalgebras since \( \mathcal{H}^0 \) is closed under \( \shuffle \) and \( \ast \). The pair \( (\mathcal{H}^1, \mathcal{H}^0) \) of spaces satisfies the polynomial ring property in one variable: the former is freely generated by \( y \) over the latter on each of \( m \) and \( \ast \). We thus have

\[
\begin{array}{l}
\mathcal{H}^1_m \simeq \mathcal{H}^0_m[y], \quad \mathcal{H}^1 \ast \simeq \mathcal{H}^0[y]. \tag{2.4}
\end{array}
\]

See [29] and [17] for proofs of (2.4), respectively.

We introduce the EDS relations stated in [18, Theorem 2(v)]. Let \( \text{reg}_m \) denote a homomorphism from \( \mathcal{H}^1_m \) to \( \mathcal{H}^0_m \), which is defined by taking the constant term with respect to \( y \) in the first isomorphism of (2.4):

\[
\text{reg}_m : \mathcal{H}^1_m \ni w = \sum_{i=0}^{m} w_i \shuffle y^m \longrightarrow w_0 \in \mathcal{H}^0. \tag{2.5}
\]

\textsuperscript{4}https://github.com/machide-tomoyan/BMZS-calculator

\textsuperscript{5}The homomorphism \( \text{reg}_m \), of stuffle type exists as well, but it is intractable because EDS relations of that type are not always \( \mathbb{Z} \)-linear: see [18] (or [1, 19]) for details.
Let \( \hat{I}_k = I_k \cup \{(1, \ldots, 1)\} \), and let

\[
\hat{\Pi}_k = \bigcup_{i,j \geq 0 \atop (i+j=k)} I_i \times I_j.
\]

For any pair \((k,l)\) of multi-indices in \(\hat{\Pi}_k\), we define

\[
ds(k,l) := \text{reg}_\text{sm}(z_k \ast z_l) - \text{reg}_\text{sm}(z_k \triangleright z_l) \in \delta^0.
\]

The objective EDS relations of weight \(k\) are stated as

\[
Z(ds(k,l)) = 0 \quad ((k,l) \in \hat{\Pi}_k),
\]

where \(Z : \delta^0 \to \mathbb{R}\) is the \(\mathbb{Q}\)-linear map (or evaluation map) defined by \(Z(z_k) = \zeta(k) (k \in I)\). We have by (2.5)

\[
\text{reg}_\text{sm}(w) = w \quad (w \in \delta^0),
\]

\[
\text{reg}_\text{sm}(y^m \triangleright z_m) = 0 \quad (m > 0, m \in I).
\]

We can thus divide (2.7) into two parts:

\[
\begin{align*}
Z(z_k \ast z_l) - Z(z_k \triangleright z_l) &= 0 \quad ((k,l) \in \hat{\Pi}_k), \\
Z(\text{reg}_\text{sm}(y^m \ast z_m)) &= 0 \quad (0 < m < k - 1, m \in I_{k-m}),
\end{align*}
\]

where \(\hat{\Pi}_k = \bigcup_{i,j \geq 0 \atop (i+j=k)} I_i \times I_j\). The relations in (2.8) are called the finite double shuffle (FDS) relations, because MZVs are defined by \(\zeta(k_1, \ldots, k_r) = \sum_{m_1 > \ldots > m_r \geq 0} 1/m_1^{k_1} \cdots m_r^{k_r}\) and finite (or convergent) at \(k \in I\). The FDS relations do not suffice to give all relations of MZVs. For instance, we can not obtain any relation in weight 3, in particular, the simplest formula \(\zeta(2,1) = \zeta(3)\). Therefore the relations in (2.9) are essential to the EDS conjecture.

A little more notions are required for (2.1), which are analogs of the notions mentioned above in \(\mathbb{Z}\)-module and \(\mathbb{F}_2\)-vector. Let \(\delta^Z\) denote the subring \(\mathbb{Z}(x,y)\) in \(\mathbb{Q}(x,y)\). We set \(\delta^Z\) to define a canonical map from \(\delta^Z\) to \(\mathcal{H}^b\) which is induced by modulo 2 arithmetic:

\[
\text{can}^b : \delta^Z \ni w = \sum_{k \in I} c_k z_k \mapsto \sum_{k \in I} (c_k \mod 2) y^b(k) \in \mathcal{H}^b.
\]

For any pair \((k,l) \in \hat{\Pi}_k\), the elements \(z_k \ast z_l\) and \(z_k \triangleright z_l\) belong to \(\delta^Z\), and the element \(\text{can}^b(ds(k,l))\) is well-defined. For \(0 < m < k - 1\) and \(m \in I_{k-m}\), \(y^m \ast z_m\) belongs to \(\langle y^n z_n \mid n \geq 0, n \in I \rangle_{\mathbb{Z}}\), and \(\text{can}^b(\text{reg}_\text{sm}(y^m \ast z_m))\) is well-defined if

\[
\text{reg}_\text{sm}(y^n z_n) \in \delta^Z \quad (n > 0, n \in I),
\]

which holds by [18, Proposition 8] (see (4.7) below). Consequently,

\[
\mathcal{E}^b_k := \langle \text{can}^b(ds(k,l)) \mid (k,l) \in \hat{\Pi}_k \rangle_{\mathbb{F}_2} \subset \mathcal{H}^b_k
\]

is well-defined.

We are in a position to define (2.1).
Table 1: EDS relations in $\mathcal{Z}_k$ and $\mathcal{Z}_k^b$ for weights $k \leq 4$.

| $k, l$ | Original EDS relation (over $\mathbb{Z}$) | Binary EDS relation (over $\mathbb{F}_2$) |
|--------|------------------------------------------|------------------------------------------|
| (1), (2) | $-\zeta(2, 1) + \zeta(3) = 0$           | $\zeta^b(2, 1) + \zeta^b(3) = 0$          |
| (1), (3) | $-\zeta(2, 2) - \zeta(3, 1) + \zeta(4) = 0$ | $\zeta^b(2, 2) + \zeta^b(3, 1) + \zeta^b(4) = 0$ |
| (1), (2, 1) | $-\zeta(2, 1, 1) + \zeta(2, 2) + \zeta(3, 1) = 0$ | $\zeta^b(2, 1, 1) + \zeta^b(2, 2) + \zeta^b(3, 1) = 0$ |
| (1, 1), (2) | $\zeta(2, 1, 1) - \zeta(2, 2) - \zeta(3, 1) = 0$ | $\zeta^b(2, 1, 1) + \zeta^b(2, 2) + \zeta^b(3, 1) = 0$ |
| (2), (2) | $-4\zeta(3, 1) + \zeta(4) = 0$           | $\zeta^b(4) = 0$                          |

**Definition 2.1.** For a weight $k$, we define the formal multiple zeta space by

$$\mathcal{Z}_k^b := \mathcal{H}_k^b / \mathcal{E}_k^b.$$ (2.11)

For a multi-index $k \in \mathbb{I}_k$, we denote by $\zeta^b(k)$ the element in $\mathcal{Z}_k^b$ which is congruent to $\eta^b(k)$ modulo $\mathcal{E}_k^b$. We call $\zeta^b(k)$ a binary multiple zeta symbol or a binary MZS.

Let $H^b$ denote the natural homomorphism from $\bigoplus_{k \geq 0} \mathcal{H}_k^b$ to $\bigoplus_{k \geq 0} \mathcal{Z}_k^b$: each component is the canonical map of (2.11). We define the binary evaluation map by $Z^b = H^b \circ \text{can}^b$. The binary EDS relations of weight $k$ are then stated as

$$Z^b(ds(k, l)) = 0 \quad ((k, l) \in \hat{\Pi}_k).$$ (2.12)

We list some examples of the original and binary EDS relations for weights $k \leq 4$ in Table 1.

Let $Z^b_{k,r}$ denote the vector subspace $\langle \zeta^b(k) \mid k \in \mathbb{I}_k, d(k) \leq r \rangle_{\mathbb{F}_2}$ as introduced in the first section. We end this section with the definition of the graded pieces satisfying the direct sum decomposition (1.5).

**Definition 2.2.** For a weight $k$, we define the depth graded formal multiple zeta spaces by

$$\mathcal{Z}_k^b := \mathcal{Z}_{k,r} / \mathcal{Z}_{k,r-1}$$ (2.13)

where $\mathcal{Z}_{k,-1} = \{0\}$.

3 Computational result

We report our computational results. How we obtain them will be explained in the next section.

We begin with a typical result related to (1.2).

**Experiment 3.1.** For any weight $k$ with $2 \leq k \leq 22$, we verify $\zeta^b(I_k^H)$ is a basis of $\mathcal{Z}_k^b$, and

$$\dim_{\mathbb{F}_2} Z^b_k = 2^{k-2} - \dim_{\mathbb{F}_2} \mathcal{E}_k^b = d_k.$$ (3.1)

The EDS conjecture states that, for every weight $k$, the relations in (2.7) suffice to reduce the number of generators of $\mathcal{Z}_k$ to $d_k$:

$$\dim_{\mathbb{Q}} \mathcal{E}_k \geq 2^{k-2} - d_k.$$ (3.2)
where $\mathcal{E}_k = \langle ds(k, l) | (k, l) \in \mathcal{PI}_k \rangle_{\mathbb{Q}}$. This can be confirmed by Experiment 3.1, as follows. We denote by $\mathcal{E}^Z_k = \langle ds(k, l) | (k, l) \in \mathcal{PI}_k \rangle_{\mathbb{Z}}$ the $\mathbb{Z}$-module counterpart of $\mathcal{E}_k$. Since $\mathbb{Q}$ is the field of fractions of $\mathbb{Z}$ and $\operatorname{can}_b$ is a surjective homomorphism from $\mathcal{E}^Z_k$ to $\mathcal{E}^b_k$, 

$$\dim_{\mathbb{Q}} \mathcal{E}_k = \operatorname{rank}_{\mathbb{Z}} \mathcal{E}^Z_k \geq \dim_{\mathbb{Z}} \mathcal{E}^b_k,$$

which, together with (3.1), proves (3.2) for $k \leq 22$. 

We recall $d^b_{k,r} = \binom{k - 2}{r - 2}$ that is the number of the Hoffman mult-indices of weight $k$ and depth $r$. We define $\mathcal{H}^b_{k,r} = \langle \eta^b(k) | k \in \mathcal{I}_k, d(k) \leq r \rangle_{\mathbb{Z}} \subset \mathcal{H}_k$, and 

$$\mathcal{E}^b_{k,r} = (\mathcal{H}^b_{k,r} \cap \mathcal{E}^b_k)/\mathcal{H}^b_{k,r-1}.$$

The main result is a refinement of Experiment 3.1. Taking the sum for $r = 1, \ldots, k - 1$ in (3.3) induces (3.1) because of (1.5): note that $\mathcal{E}^b_{k,0} = \{0\}$ unless $k = 0$. 

**Experiment 3.2.** For any weight $k$ and depth $r$ with $1 \leq r < k \leq 22$, we verify $\mathcal{E}^b_k(\mathcal{I}^H_{k,r})$ is a basis of $\mathcal{E}^b_{k,r}$, and 

$$\dim_{\mathbb{Z}} \mathcal{E}^b_{k,r} = \binom{k - 2}{r - 1} - \dim_{\mathbb{Z}} \mathcal{E}^b_{k,r} = d^b_{k,r}. \quad (3.3)$$

The first equality in (3.3) is by the isomorphism theorems. In fact, we have 

$$\mathcal{Z}^b_{k,r}/\mathcal{Z}^b_{k,r-1} \simeq \mathcal{H}^b_{k,r}/(\mathcal{H}^b_{k,r} \cap \mathcal{E}^b_k) \bigg/ \mathcal{H}^b_{k,r-1}/(\mathcal{H}^b_{k,r-1} \cap \mathcal{E}^b_k)$$

$$\simeq \mathcal{H}^b_{k,r}/(\mathcal{H}^b_{k,r-1} + \mathcal{H}^b_{k,r} \cap \mathcal{E}^b_k)$$

$$\simeq \mathcal{H}^b_{k,r}/\mathcal{H}^b_{k,r-1} \big/ (\mathcal{H}^b_{k,r} \cap \mathcal{E}^b_k)/\mathcal{H}^b_{k,r-1}. \quad (3.4)$$

and 

$$\mathcal{Z}^b_{k,r} \simeq \mathcal{H}^b_{k,r}/\mathcal{H}^b_{k,r-1}/\mathcal{E}^b_{k,r}.$$ 

Since $\binom{k - 2}{r - 1} = |\mathcal{H}^b_{k,r}/\mathcal{H}^b_{k,r-1}|$ by counting the number of the mult-indices of weight $k$ and depth $r$, we obtain the desired equality.

We demonstrate the numbers $d^b_{k,r}$ for $k \leq 22$ in Table 2. They are expressed in terms of binomial coefficients, and we can observe a (shifted) Pascal triangle pattern: the column $r = 0$ has the sequence (1) from the row $k = 0$, the column $r = 1$ has (1, 1) from $k = 2$, the column $r = 2$ has (1, 2, 1) from $k = 4$, the column $r = 3$ has (1, 3, 3, 1) from $k = 6$, and so on. For comparison, the dimensions of $\mathcal{Z}_{k,r}$ conjectured in (1.8) are listed in Table 3.

Refinements of the EDS conjecture have been proposed. Minh et al. [26] conjectured that a part of the EDS relations obtained from 

$$\widehat{\mathcal{PI}}^\text{MPO}_{\mathcal{I}k} = \mathcal{PI}_{\mathcal{I}k} \cup \widehat{(\mathcal{I}_1 \times \mathcal{I}_{k-1})} \quad (3.5)$$

is a right candidate, and verified it up to $k = 16$. The relations 

$$Z(ds(k, l)) = 0 \quad ((k, l) \in \widehat{(\mathcal{I}_1 \times \mathcal{I}_{k-1})})$$

are known as Hoffman’s relations ([17]), and their conjecture says that FDS relations and Hoffman’s relations suffice to give all relations among MZVs. Kaneko et al. [20] conjectured the above relations are too much, i.e., a smaller part obtained from 

$$\widehat{\mathcal{PI}}^\text{KNT}_{\mathcal{I}k} = \{(3, (2, 1)) \times \mathcal{I}_{k-3}\} \cup \{(2) \times \mathcal{I}_{k-2}\} \cup \widehat{(\mathcal{I}_1 \times \mathcal{I}_{k-1})} \quad (3.6)$$

7
Table 2: The numbers $d_{k,r}^b$ for $0 \leq r < k \leq 22$: the unlisted numbers $d_{k,r}^b$ ($r > 11$) are 0. The total number of each row is $d_k$ and that of each column is $2^r$ (for $r \leq 7$).

| $k/r$ | 0  | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | Total |
|-------|----|----|----|----|----|----|----|----|----|----|----|----|-------|
| 0     | 1  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 1     |
| 1     | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0     |
| 2     | 0  | 1  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 1     |
| 3     | 0  | 1  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 1     |
| 4     | 0  | 0  | 1  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 1     |
| 5     | 0  | 0  | 2  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 2     |
| 6     | 0  | 0  | 1  | 1  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 2     |
| 7     | 0  | 0  | 0  | 3  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 3     |
| 8     | 0  | 0  | 0  | 3  | 1  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 4     |
| 9     | 0  | 0  | 0  | 1  | 4  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 5     |
| 10    | 0  | 0  | 0  | 0  | 6  | 1  | 0  | 0  | 0  | 0  | 0  | 0  | 7     |
| 11    | 0  | 0  | 0  | 0  | 4  | 5  | 0  | 0  | 0  | 0  | 0  | 0  | 9     |
| 12    | 0  | 0  | 0  | 0  | 1  | 10 | 1  | 0  | 0  | 0  | 0  | 0  | 12    |
| 13    | 0  | 0  | 0  | 0  | 0  | 10 | 6  | 0  | 0  | 0  | 0  | 0  | 16    |
| 14    | 0  | 0  | 0  | 0  | 0  | 5  | 15 | 1  | 0  | 0  | 0  | 0  | 21    |
| 15    | 0  | 0  | 0  | 0  | 0  | 1  | 20 | 7  | 0  | 0  | 0  | 0  | 28    |
| 16    | 0  | 0  | 0  | 0  | 0  | 0  | 15 | 21 | 1  | 0  | 0  | 0  | 37    |
| 17    | 0  | 0  | 0  | 0  | 0  | 0  | 6  | 35 | 8  | 0  | 0  | 0  | 49    |
| 18    | 0  | 0  | 0  | 0  | 0  | 0  | 1  | 35 | 28 | 1  | 0  | 0  | 65    |
| 19    | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 21 | 56 | 9  | 0  | 0  | 86    |
| 20    | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 7  | 70 | 36 | 1  | 0  | 114   |
| 21    | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 1  | 56 | 84 | 10 | 0  | 151   |
| 22    | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 0  | 28 | 126 | 45 | 1  | 200   |
| Total | 1  | 2  | 4  | 8  | 16 | 32 | 64 | 128| −  | −  | −  | −  | −     |

is a right candidate. They verified it up to $k = 20$.

In the space $\mathcal{Z}_k^b$, neither the relations obtained from (3.5) nor those obtained from (3.6) suffice to give all relations among binary MZSs.

**Experiment 3.3.** Let $\bullet \in \{\text{KNT}, \text{MJPO}\}$ and let $\mathcal{E}_k^b \bullet = \langle \text{can}^b(ds(k, l)) \mid (k, l) \in \widehat{\text{PI}}^b_{k} \rangle_{F_2}$. There exist weights $k \leq 22$ such that

$$\dim_{F_2} \mathcal{E}_k^b \bullet < 2^{k-2} - d_k.$$  \hspace{1cm} (3.7)

Computational results of $d_k^b \bullet = 2^{k-2} - \dim \mathcal{E}_k^b \bullet$ are shown in Table 4. In general,

$$d_k^{b, \text{KNT}} > d_k^{b, \text{MJPO}} > d_k.$$  \hspace{1cm} (3.8)

We can find that the sequence $(d_{k}^{b, \text{MJPO}})_{0 \leq k \leq 22}$ has a quasi Fibonacci-like rule,

$$d_k^{b, \text{MJPO}} = d_{k-2}^{b, \text{MJPO}} + d_{k-3}^{b, \text{MJPO}} + \delta_{M,k},$$  \hspace{1cm} (3.8)

where $M = \{7, 15\}$ and $\delta_{M,k}$ is the Kronecker delta function defined by $\delta_{M,k} = 1$ if $k \in M$ and $\delta_{M,k} = 0$ otherwise. It appears that $(d_{k}^{b, \text{KNT}})_{0 \leq k \leq 22}$ does not have an obvious law.
Table 3: The conjectural numbers $\dim \mathbb{Z}_{k,r}$ for $0 \leq r < k \leq 22$: the unlisted numbers $\dim \mathbb{Z}_{k,r}$ for $r > 11$ are 0.

| $k/r$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | Total |
|-------|---|---|---|---|---|---|---|---|---|---|-----|-----|-------|
| 0     | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 1     |
| 1     | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 0     |
| 2     | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 1     |
| 3     | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 1     |
| 4     | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 1     |
| 5     | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 2     |
| 6     | 0 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 2     |
| 7     | 0 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 3     |
| 8     | 0 | 1 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 4     |
| 9     | 0 | 1 | 3 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 5     |
| 10    | 0 | 1 | 3 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 7     |
| 11    | 0 | 1 | 4 | 3 | 1 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 9     |
| 12    | 0 | 1 | 3 | 6 | 2 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 12    |
| 13    | 0 | 1 | 5 | 6 | 4 | 0 | 0 | 0 | 0 | 0 | 0   | 0   | 16    |
| 14    | 0 | 1 | 5 | 9 | 4 | 2 | 0 | 0 | 0 | 0 | 0   | 0   | 21    |
| 15    | 0 | 1 | 6 | 8 | 10 | 3 | 0 | 0 | 0 | 0 | 0   | 0   | 28    |
| 16    | 0 | 1 | 5 | 14 | 11 | 6 | 0 | 0 | 0 | 0 | 0   | 0   | 37    |
| 17    | 0 | 1 | 7 | 13 | 18 | 7 | 3 | 0 | 0 | 0 | 0   | 0   | 49    |
| 18    | 0 | 1 | 6 | 19 | 18 | 17 | 4 | 0 | 0 | 0 | 0   | 0   | 65    |
| 19    | 0 | 1 | 8 | 17 | 31 | 19 | 10 | 0 | 0 | 0 | 0   | 0   | 86    |
| 20    | 0 | 1 | 7 | 25 | 30 | 35 | 12 | 4 | 0 | 0 | 0   | 0   | 114   |
| 21    | 0 | 1 | 9 | 22 | 48 | 37 | 29 | 5 | 0 | 0 | 0   | 0   | 151   |
| 22    | 0 | 1 | 8 | 32 | 45 | 65 | 33 | 16 | 0 | 0 | 0   | 0   | 200   |

4 Computer program

Our computer programs, that perform the Gaussian forward elimination on the linear combinations in $\mathcal{E}_k^b$, show the following proposition.

**Proposition 4.1.** Let $k$ and $r$ be a weight and depth, respectively, with $r < k \leq 22$. For a multi-index $k$ in $I_{k,r}$, the following statements hold.

(i) If $k \notin I_{k,r}^H$, there exists a combination $c \in \mathcal{H}_{k,r}^b \cap \mathcal{E}_k^b$ such that

\[ \eta^b(k) \in c + \langle \eta^b(h) \mid h \in I_{k,r}^H \cup I_{k,r-1}^H \cup \cdots \cup I_{k,\lfloor k/3 \rfloor}^H \rangle_{\mathbb{F}_2}. \]  

(ii) If $k \in I_{k,r}^H$, there exists no combination $c$ such as (4.1).

Here $\lfloor \cdot \rfloor$ is the floor function defined by $\lfloor t \rfloor = \max \{ a \in \mathbb{Z} \mid a \leq t \}$ for a real number $t$.

Proposition 4.1 verifies Experiment 3.2. Suppose $k \in I_{k,r} \setminus I_{k,r}^H$. By the statement (i),

\[ \zeta^b(k) \in \langle \zeta^b(h) \mid h \in I_{k,r}^H \cup I_{k,r-1}^H \cup \cdots \cup I_{k,\lfloor k/3 \rfloor}^H \rangle_{\mathbb{F}_2}, \]  

or

\[ \gamma^b(k) \in \langle \gamma^b(h) \mid h \in I_{k,r}^H \rangle_{\mathbb{F}_2}, \]
Table 4: The numbers \(d_k^b\bullet (\bullet \in \{\text{KNT, MJPO}\})\) with \(d_k\): they are same when \(k \leq 6\).

| \(k\) | \(d_k^b\text{KNT}\) | \(d_k^b\text{MJPO}\) | \(d_k\) |
|-------|------------------|------------------|--------|
| 7     | 4                | 4                | 3      |
| 8     | 6                | 4                | 4      |
| 9     | 8                | 6                | 5      |
| 10    | 12               | 8                | 7      |
| 11    | 21               | 10               | 9      |
| 12    | 30               | 14               | 12     |
| 13    | 44               | 18               | 16     |
| 14    | 66               | 24               | 21     |
| 15    | 100              | 33               | 28     |
| 16    | 140              | 42               | 37     |
| 17    | 208              | 57               | 49     |
| 18    | 300              | 75               | 65     |
| 19    | 441              | 99               | 86     |
| 20    | 644              | 132              | 114    |
| 21    | −                | 174              | 151    |
| 22    | −                | 231              | 200    |

which, together with the statement (ii), implies \(\zeta^b(\mathbf{H}_{k,r}^b)\) is a basis of \(\mathbb{Z}_{k,r}^b\) for \(r < k \leq 22\).

Imaginarily, the Gaussian elimination can elucidate any vector space whose corresponding matrix (or set of defining linear combinations) is clearly given: but practically, it is limited to a space that are not too big. The bound \(k = 22\) in Proposition 4.1 indicates a performance threshold of our computing environments. Below we will describe the environments and prove Proposition 4.1.

The programs are written almost by Python language and partly by Cython language. The machine is as follows: a Linux-based PC having two CPUs with 12-core at 2.70GHz (Intel Xeon Gold 6226) and a 3TB RAM. The package of the programs is available at https://github.com/machide-tomoyan/BMZS-calculator.

The executable files are in the directories named as Main_make and Main_cal. The former contains five files that produce datas of binary systems (or binary matrices) obtained from the binary EDS relations, and the latter contains one file that calculates dimensions of \(\mathbb{Z}_k^b\) and \(\mathbb{Z}_{k,r}^b\) (or row echelon forms of the corresponding binary matrices). The produced datas are stocked in Data, almost of which are saved in Python pickle format to reduce data size. Class files in which essential precesses are performed are stored in Work. Files of config, license and readme are also placed in the root directory of the package. (See Figure 1 for a layout of the package).

We have a convenient expression for a linear combination in \(\mathbb{Z}_k^b\) since \(\mathbb{F}_2\) consists of only two elements. A subset \(\mathbf{J}\) in \(\mathbf{I}_k\) is identified with a combination such as

\[
\mathbf{J} \leftrightarrow \sum_{k \in \mathbf{J}} \zeta^b(k). \tag{4.4}
\]

For instance, \(\mathbf{J}_1 = \{(2, 1, 1), (2, 2), (3, 1)\}\) corresponds to \(\zeta^b(2, 1, 1) + \zeta^b(2, 2) + \zeta^b(3, 1)\) and \(\mathbf{J}_2 = \{(2, 2), (3, 1), (4)\}\) corresponds to \(\zeta^b(2, 2) + \zeta^b(3, 1) + \zeta^b(4)\). By (4.4), the symmetric difference \(\triangle\) of two sets is equivalent to the plus of two combinations: \(\mathbf{J}_1 \triangle \mathbf{J}_2 = (\mathbf{J}_1 \setminus
Figure 1: Layout of our package for the executable files.

\[ J_2 \cup (J_2 \setminus J_1) = \{(2,1,1),(4)\} \] corresponds to \((\zeta^b(2,2) + \zeta^b(3,1) + \zeta^b(4)) + (\zeta^b(2,1,1) + \zeta^b(2,2) + \zeta^b(3,1)) = \zeta^b(2,1,1) + \zeta^b(4)\). The expression (4.4) is also applied to a linear relation \(\sum_{k \in J} \zeta^b(k) = 0\) in the same way. We compute binary EDS relations (or defining combinations in \(E_b^k\)) through (4.4) with the set datatype in Python. This set based expression can be realized by built-in objects.\(^6\)

We will explain the executable files and report their statics. We do not mention actual command lines to use the files in a linux OS, but we can find them in the beginning of each file.

4.1 Executable file in \texttt{Main make}

We will require many maps to save midway datas for the binary linear systems induced from the binary EDS relations. The prime reason is that, by (2.6), each EDS relation is composed of a combination of \(\ast\) and \(\text{reg}\). For the maps or the midway datas, we will use dictionary datatype, which is a built-in object in Python and consists of a collection of tuples of two objects called ‘key’ and ‘value’: a key-object is mapped to its associated value-object.

The file \texttt{0.preparation.py} prepares two dictionary datas for each weight \(k \leq 22\). Let \([n]\) denote the set \(\{1, \ldots, n\}\) for a positive integer \(n\). One data gives a one-to-one mapping from the integers in \([2^k]\) to the words of degree \(k\), and another data gives a one-to-one mapping from the integers in \([2^{k-1}]\) to the mult-indices in \(\bigcup_{r=1}^{k} N_r\) of weight \(k\): if \(n \in [2^{k-1}]\) and the associated mult-index is \(k\), the associated word is \(z_k\). The objects of the set which our programs select for the set based expression in the left of (4.4) are the integers (for which the integer datatype is necessary) instead of the mult-indices and words (for which the tuple and string datatypes are necessary), because the integer datatype is reasonable in data size and running time.

The file \texttt{1.product.py} creates dictionary datas for shuffle and stuffle products. The defining equations (2.2) and (2.3) suggest that creating datas of shuffle will take more time since shuffle products can contain more terms. For a speed-up, we improve (2.2):

\[
\begin{align*}
  a_1 \cdots a_m \Uparrow b_1 \cdots b_n &= \sum_{0 \leq i < j \leq \min(t,m) \atop 0 \leq l \leq \min(t,n)} (a_1 \cdots a_i \Uparrow b_1 \cdots b_j) (a_{i+1} \cdots a_m \Uparrow b_{j+1} \cdots b_n),
\end{align*}
\]

\(^6\)We use \texttt{frozenset} and \texttt{s.symmetric_difference(t)} (or the operator notation ‘s \^{\_} t’), where \texttt{frozenset} is an immutable datatype for set datas and \texttt{s,t} are its instances.
where \( a_1, \ldots, a_m, b_1, \ldots, b_n \in \{x, y\} \) and \( 0 < l \leq m + n \). This is a special case of (2.2) if \( l = 1 \) and can be proved by induction on \( l \). Let \( k = m + n \). Using (4.5) with \( l = \lfloor k/2 \rfloor \), we can reduce shuffle products of weight \( k \) to combinations of those of about half weight.

We denote by \( \text{Sh} \) and \( \text{St} \) created datas of shuffle and stuffle, respectively. They map pairs of words that cannot be written in terms of mult-indices (e.g., \( z \), \( x \), \( y \)) to combinations of those of about half weight.

\[
\text{Sh}((1), (2)) = \zeta^b_m(1, 2), \\
\text{St}((1), (2)) = \zeta^b_m(1, 2) + \zeta^b(2, 1) + \zeta^b(3),
\]

(4.6)

In the case of shuffle, for using (4.5) with \( l = \lfloor k/2 \rfloor \), we also create maps from pairs of words to combinations of words up to weight \( 22/2 = 11 \). In those additional maps, we allow the words that cannot be written in terms of mult-indices (e.g., \( x, y \) and \( yx = z_1x \)).

Let \( k \) be a mult-index that is expressed as \( z_k = y^n z_n \), where \( n \geq 0 \) and \( n \in I \setminus \{\emptyset\} \). Let \( n' \) denote a mult-index such that \( z_n = x z_{n'} \). By [18, Proposition 8],

\[
\text{reg}_{mn}(y^n z_n) = (-1)^n x(y^n m z_{n'}). \tag{4.7}
\]

Since the regularized MZV of \( z_k \) is \( Z \circ \text{reg}_{mn}(y^n z_n) \), its binary version should be

\[
\zeta^b_m(k) = Z^b \circ \text{reg}_{mn}(y^n z_n) = H^b \circ \text{can}^b(x(y^n m z_{n'})). \tag{4.8}
\]

The dictionary datas that the file `2_regularized_product.py` creates are obtained by applying (4.8) to ones that the previous file creates. For instance, we have by (4.8)

\[
\zeta^b_m(1, 2) = H^b \circ \text{can}^b(x(y m y)) = H^b(\text{can}^b(2xyy)) = 0,
\]
\[
\zeta^b_m(1, 1, 2) = H^b \circ \text{can}^b(x(y^2 m y)) = H^b(\text{can}^b(3xyyy)) = \zeta^b(2, 1, 1),
\]
\[
\zeta^b_m(1, 2, 1) = H^b \circ \text{can}^b(x(y m yy)) = H^b(\text{can}^b(3xyy)) = \zeta^b(2, 1, 1),
\]
\[
\zeta^b_m(1, 1, 3) = H^b \circ \text{can}^b(x(y m xy)) = H^b(\text{can}^b(xyxy + 2xxyy)) = \zeta^b(2, 2),
\]

and so the previous datas in (4.6) are converted to

\[
\text{Sh}_m((1), (2)) = 0, \\
\text{St}_m((1), (2)) = \zeta^b(2, 1) + \zeta^b(3), \\
\text{Sh}_m((1, 1), (2)) = 0, \\
\text{St}_m((1, 1), (2)) = \zeta^b(2, 1, 1) + \zeta^b(2, 2) + \zeta^b(3, 1),
\]

(4.9)

where \( \text{Sh}_m \) and \( \text{St}_m \) stand for the maps of regularized shuffle and stuffle, respectively.

The file `3_extended_relation.py` makes binary EDS relations,

\[
\text{St}_m(k, l) + \text{Sh}_m(k, l) = 0 \quad ((k, l) \in \mathbf{\Pi}_k),
\]

by combining the previous datas. For instance, the datas in (4.9) create the two relations,

\[
\zeta^b(2, 1) + \zeta^b(3) = 0,
\]
\[
\zeta^b(2, 1, 1) + \zeta^b(2, 2) + \zeta^b(3, 1) = 0.
\]

The file `4_binary_system.py` converts the binary EDS relations of a weight \( k \) to a binary linear system (which we call a binary EDS linear system) in both of text and pickle formats. The text format is organized as follows:
Table 5: Elapsed real times [sec] to make binary systems.

| $k$ | $0_{\text{M.py}}$ | $1_{\text{M.py}}$ | $2_{\text{M.py}}$ | $3_{\text{M.py}}$ | $4_{\text{M.py}}$ | Total |
|-----|-------------------|-------------------|-------------------|-------------------|-------------------|-------|
| 18  | 0                 | 75                | 246               | 53                | 54                | 428 ($\approx$ 7min) |
| 19  | 1                 | 188               | 805               | 133               | 186               | 1313 ($\approx$ 22min) |
| 20  | 3                 | 469               | 3137              | 510               | 543               | 4662 ($\approx$ 1.3hour) |
| 21  | 7                 | 1529              | 15607             | 1384              | 2362              | 20889 ($\approx$ 5.8hour) |
| 22  | 15                | 3018              | 61898             | 3675              | 6578              | 75184 ($\approx$ 21hour) |

1. A line with the first character ‘#’ is a comment line. Comment lines typically occur at the beginning of the file, but are allowed to appear throughout the file.

2. The remainder of the file contains lines defining the binary linear relations, one by one.

3. A relation is defined by positive integers numbering binary MZSs. A number ‘0’ is typically placed at the last of the line, but it is optional.

For example, the line “2 4 0” is corresponding to $\zeta^b(2, 1) + \zeta^b(3) = 0$, if $\zeta^b(2, 1)$ and $\zeta^b(3)$ are numbered as 2 and 4, respectively. The pickle files are not necessary but useful: e.g., when loading the large size system. For Experiment 3.3, we also make binary KNT and MJPO linear systems by restricting binary EDS relations.

The above programs run under the parallel process since the datas can be created independently if $\hat{\Pi}_k$ is divided into a plurality of blocks. The filenames of the datas by the parallel process have strings ‘$\_Bn$ ($n \in \mathbb{N}$) at their tails. Editing the file config.txt we can control the max number of parallel threads.

In Table 5, we present computation times (or elapsed real times) to execute all files for $k \geq 18$, where $i_{\text{M.py}}$ stands for the $i$-th file mentioned above from 0 to 4. We find that calculating the regularizations in $2_{\text{M.py}}$ is the dominant process. Table 6 lists the file sizes of the binary linear systems in pickle format for $\hat{\Pi}^{\text{KNT}}_k$, $\hat{\Pi}^{\text{MJPO}}_k$, and $\hat{\Pi}^{\text{EDS}}_k$. As expected from $\hat{\Pi}^{\text{KNT}}_k \subset \hat{\Pi}^{\text{MJPO}}_k \subset \hat{\Pi}^{\text{EDS}}_k$, the file of KNT is smallest and that of EDS is largest for each weight. The size of text format file is about 1.5 times the size of pickle one. For each weight $k$, the maximum memory size (or maximum resident set size) to execute the files $i_{\text{M.py}}$ is the size required by $4_{\text{M.py}}$, which is about half size used in Gaussian forward elimination (see Table 7). Computationally, making linear systems is not harder than calculating their coranks (or dimensions of cokernel) as we will see below.

4.2 Executable file in Main_cal

The file dimensions.py (d_C.py for short) executes the Gaussian forward elimination on a given binary linear system of a weight $k$ by using Algorithm A.6. In the process, an order of mult-indices (or binary MZSs) have to be determined to convert the inputted binary linear system into the corresponding binary matrix. We employ a sequence $(k_1, \ldots, k_{2^k-2})$ satisfying the following: if $i < j$,

(a) $d(k_i) > d(k_j)$; or
(b) $d(k_i) = d(k_j)$ and $(k_i, k_j) \notin \mathbf{I}_k^H \times (\mathbf{I}_k \setminus \mathbf{I}_k^H)$. 

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Table 6: File sizes of binary linear systems in pickle format.

| \(k\) | KNT | MJPO | EDS |
|-------|-----|------|-----|
| 18    | 8.3M| 150M | 274M|
| 19    | 21M | 509M | 922M|
| 20    | 47M | 1.6G | 2.8G|
| 21    | 105M| 5G   | 8.6G|
| 22    | 233M| 16G  | 26G |

The condition (a) means that the multi-indices (or columns in the corresponding matrix) are sectioned into \(k - 1\) blocks by depth: the multi-indices in a left block have a greater depth than those in a right block. The condition (b) means that the Hoffman multi-indices of depth \(r\) are at the rightmost place in the \((k - r)\)th block. For example, the order of weight 4 determined by \(k_1 = (2, 1, 1), k_2 = (3, 1), k_3 = (2, 2)\) and \(k_4 = (4)\) satisfies (a) and (b): they are sectioned as \((k_1)\|(k_2, k_3)\|(k_4)\) and the only Hoffman multi-index \(k_3\) is located rightmost in the 2th block.

Proposition 4.1 is shown as follows.

Proof of Proposition 4.1. We consider the situation where we run \(\text{d}_C\text{.py}\) by inputing the binary EDS linear system of weight \(k\). We then obtain a row echelon matrix satisfies the following.

(E1) There exists a non-zero pivot at any column \(k\) in \(I_k \setminus I^H_k\).

(E2) There exists no non-zero pivot at any column \(k\) in \(I^H_k\).

For a non-zero combination \(c = \eta^b(k_{i_1}) + \cdots + \eta^b(k_{i_j})\) in \(H^b_k\) with \(i_1 < \cdots < i_j\), we define the leading term of \(c\) by

\[ L(c) = \eta^b(k_{i_1}) \].

By (a) and (b), the statements (E1) and (E2) are equivalent to (e1) and (e2), respectively:

(e1) There exists a combination \(c \in E^b_k\) such that \(L(c) = \eta^b(k)\) for any \(k\) in \(I_k \setminus I^H_k\).

(e2) There exists no combination \(c \in E^b_k\) such that \(L(c) = \eta^b(k)\) for any \(k\) in \(I^H_k\).

Under (e1) and (e2), the back substitution (performed imaginarily) implies Proposition 4.1, where the fact that \(I^H_{k,r} = \phi\) for any depth \(r < \lfloor k/3 \rfloor\) is used for (4.1).

We give examples of (4.3) for \(k \leq 7\) excluding the case that \(\zeta^b(k) = 0\). Note that \(\zeta^b(k)\) is always zero if \(k \in I_{k,r}\) and \(I^H_{k,r} = \phi\).

\[
\zeta^b(3, 1) = \zeta^b(2, 2),
\]
\[
\zeta^b(4, 1) = \zeta^b(2, 3) + \zeta^b(3, 2),
\]
\[
\zeta^b(2, 1, 3) = \zeta^b(3, 2, 1) = \zeta^b(4, 1, 1) = \zeta^b(2, 2, 2),
\]
\[
\zeta^b(5, 1) = \zeta^b(3, 3),
\]
\begin{align*}
\zeta^a(5, 1, 1) &= \zeta^a(3, 1, 3) = \zeta^a(2, 2, 3) + \zeta^a(2, 3, 2) + \zeta^a(3, 2, 2), \\
\zeta^a(3, 1, 1) &= \zeta^a(2, 3, 2), \\
\zeta^a(4, 2, 1) &= \zeta^a(2, 2, 3) + \zeta^a(2, 3, 2), \\
\zeta^a(4, 1, 2) &= \zeta^a(2, 1, 4) = \zeta^a(2, 2, 3) + \zeta^a(3, 2, 2), \\
\zeta^a(2, 4, 1) &= \zeta^a(2, 3, 2) + \zeta^a(3, 2, 2).
\end{align*}

Examining the Gaussian forward elimination performed by \texttt{d.C.py} in detail, we can find a part of the inputted binary EDS relations which forms a basis of \( E_k^b \). We give examples of bases for \( k \leq 6 \), where only the pairs of mult-indices are written (see Table 1 that lists associated relations for \( k \leq 4 \)).

\( k = 3 \): ((1), (2)).
\( k = 4 \): ((1), (2, 1)), ((1), (3)), ((2), (2)).
\( k = 5 \): ((1), (2, 1, 1)), ((1), (2, 2)), ((1), (3, 1)), ((1), (4)), ((2), (2, 1)), ((2), (3)).
\( k = 6 \): ((1), (2, 1, 1, 1)), ((1), (2, 1, 2)), ((1), (2, 2, 1)), ((1), (2, 3)), ((1), (3, 1, 1)), ((1), (3, 2)), ((1), (4, 1)), ((1), (5)), ((2), (2, 1, 1)), ((2), (2, 2)), ((2), (3, 1)), ((2, 1), (2, 1)), ((2, 1), (3)), ((3), (3)).

We can verify Experiment 3.3 similarly to Experiment 3.2. We input KNT and MJPO linear systems into \texttt{d.C.py}. By Table 4, in most cases, row echelon matrices that do not satisfy (E1) are outputted. The fails of (E1) induce (3.7), and ensure Experiment 3.3.

The program in \texttt{d.C.py} applies the parallel process to determine an order of mult-indices since mult-indices can be divided by depth. For instance, \((k - 1)\) parallel threads occur as preprocessing if a binary EDS linear system of weight \( k \) is inputted. Algorithm A.6, the main process for computing a row echelon matrix, is executed in single. It appears that the parallelization of Algorithm A.6 is not easy because a non-simple search procedure is incorporated.

In Table 7, we present the statics of the executions by \texttt{d.C.py} whose inputs are the binary KNT, MJPO and EDS relations. We observe that the computation for KNT requires much more time than MJPO and EDS, although the number of relations of KNT is quite small such that the corresponding matrix is square for any \( k \geq 7 \). This phenomenon expresses a characteristic of Algorithm A.6. It employs a conflict based search procedure inspired by the conflict-driven clause learning (CDCL), a modern method with many successes to practical applications in solving the Boolean satisfiability (SAT) problem. Roughly speaking, relations with good structures for finding conflict combinations can accelerate searching a pivot relation (see Remark A.7 for more information). The memory cost is bad in comparison with the statics in [20], but the runtime is about 10 times more faster. Therefore we can improve the record of calculating (3.2) from \( k = 20 \) to 22 by the use of a machine with large memory capacity.

## 5 Problem

Some problems arise in connection with the experiments in Section 3.

Experiments 3.1 and 3.2 indicate typical problems on the dimensions of \( \mathbb{Z}_k^b \) and \( \mathbb{Z}_{k,r}^b \); obviously, Problem 5.2 includes Problem 5.1.
Table 7: Statistics of the computations of Experiments 3.2 and 3.3. ‘Rels’ is the number of relations. ‘MeanNum’ is the average number of terms per relation. ‘Memory’ and ‘Time’ are the resident set size and elapsed real time, respectively. In each block with respect to the weight $k$, top row indicates information on KNT, middle row indicates that on MJPO and bottom row indicates that on EDS.

| $k$ | $2^{k-2}$ | Rels | MeanNum | Memory | Time  |
|-----|-----------|------|---------|--------|-------|
| 18  | 65536     | 65536| 30.1    | 4.6G   | 8.6hour |
|     | 155711    | 230.4| 7.3G    | 8.8min |
|     | 188470    | 364.4| 11.4G   | 9.8min |
| 19  | 131072    | 131072| 33.7    | 16.5G  | 68hour |
|     | 327679    | 339.5| 22.9G   | 42.4min|
|     | 393206    | 523.1| 34.3G   | 43.7min|
| 20  | 262144    | 262144| 37.6    | 61G    | 22day  |
|     | 688254    | 500.5| 82G     | 5.3hour|
|     | 819316    | 751.7| 110G    | 4.7hour|
| 21  | 524288    | 524288| -       | -      | -      |
|     | 1441791   | 739.8| 256G    | 30hour |
|     | 1703925   | 1083.3| 329G   | 25hour |
| 22  | 1048576   | 1048576| -       | -      | -      |
|     | 3014911   | 1094.4| 789G    | 8day   |
|     | 3539188   | 1564.1| 982G    | 7day   |

Problem 5.1. Does (3.1) hold for any weight $k$?

Problem 5.2. Does (3.3) (or Proposition 4.1) hold for any weight $k$ and depth $r$?

Experiment 3.3 yields the following:

Problem 5.3. (i) Is there a subset $M \subset \mathbb{N}$ such that $M \cap \lbrack 22 \rbrack = \{7, 15\}$ and the sequence $(d_{k}^{b,\text{MJPO}})_{k \geq 0}$ satisfies (3.8)?

(ii) Can we find a law in the sequence $(d_{k}^{b,\text{KNT}})_{k \geq 0}$?

We have adopted the binary field $\mathbb{F}_2$ for the scalar field of the formal multiple zeta space and for the computation of corank. (It is worth noting that the experiments of [20] employ $\mathbb{F}_{16381}$ and $\mathbb{F}_{31991}$.) There are no particular reasons for choosing $\mathbb{F}_2$ except computational science techniques are easy to apply. A discovery of a regularity of $d_{k,r}^{b}$ in Table 2 is a product of good luck.

Problem 5.4. (i) Can we find a theoretical reason why the dimensions $d_{k,r}^{b}$ ($r < k \leq 22$) have a Pascal triangle pattern?

(ii) What will the dimensions be if we adopt other finite fields $\mathbb{F}_p$?

Like MZVs, we can make an assumption that binary MZSs satisfy a multiplication compatible with the shuffle and stuffle products. Under the assumption, we have $\zeta_{b}(2)^2 = 0$ since $Z_{b}(z_{2})Z_{b}(z_{2}) = Z_{b}(z_{2} \shuffle z_{2}) = H_{b} \circ \mathrm{can}_{b}(2z_{2} + 4z_{3,1}) = 0$. This means that the algebras of
MZV and binary MZS are different. In particular, $F_2[\zeta^b(2)] = \langle 1, \zeta^b(2) \rangle_{F_2}$ is not isomorphic to the polynomial ring in one variable, and statements and conjectures involving $F/\zeta^b(2)$, e.g., those involving finite and symmetric multiple zeta values introduced in [19]) can not be varied to $Z^b/\zeta^b(2)Z^b$ directly. It seems a mysterious problem that whether the algebra of binary MZS has a good property and a connection to the algebra of MZV.

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**Appendix**

We will introduce a technique to speed up the Gaussian forward elimination over any field $K$ for a system of linear combinations that have some structure. An essential part of the technique appears in [23] to decide the full rankness of a binary matrix.

Let $x_1, \ldots, x_n$ be variables, and we order the variables according to their subscripts. For a non-zero linear combination $p = p(x_1, \ldots, x_n) = \sum c_i x_i$ over $K$, we denote by $s_{\min}(l)$ and $c_{\min}(l)$ the subscript and coefficient of the minimum variable, respectively. That is, $s_{\min}(p) = \min \{i | c_i \neq 0\}$ and $c_{\min}(p) = c_{s_{\min}(p)}$. We define $s_{\min}(p) = n + 1$ and $c_{\min}(p) = 0$ when $p = 0$.

In what follows we will handle mainly linear combinations over $K$, and we just call them combinations. Let $K_{p_1, \ldots, p_m}$ denote the $K$-vector space spanned by combinations $p_1, \ldots, p_m$, and let $K^*_{p_1, \ldots, p_m} = K_{p_1, \ldots, p_m} \setminus \{0\}$. We say that $p_i$ is a pivot combination if $s_{\min}(p_i) = i$, and

$$(p_{i_1})_{1 \leq i \leq h} = (p_{i_1}, \ldots, p_{i_h})$$

is a pivot sequence if $1 \leq i_1 < \cdots < i_h \leq n$ and every $p_{i_g}$ is a pivot combination.

There are two key processes for the speed-up technique. One is a conflict search search procedure.

**Process A.1.**

**Input:** Combinations $L = \{l_1, \ldots, l_m\}$ and a pivot sequence $(p_1, \ldots, p_{j-1})$.

**Output:** Either $(0, \emptyset)$ or $(q_i, k_i)$ such that

(a) $q_i \in L$ with $s_{\min}(q_i) = i \leq j$;
(b) $k_i = (k_i, \ldots, k_{j-1}, k_j, \ldots, k_n) \in K^{n-i+1}$ with $k_j = 1$ and $k_{j+1} = \cdots = k_n = 0$;
(c) $q_i \mid (x_{i_1}, \ldots, x_{n}) = k_i \in K^*$; and
(d) $p_i \mid (x_{i_1}, \ldots, x_{n}) = k_i = \cdots = p_{j-1} \mid (x_{i_1}, \ldots, x_{n}) = k_i = 0$.

1. Set $k_j = (k_j, \ldots, k_n) = (1, 0, \ldots, 0) \in K^{n-j+1}$ and $i = j$.
2. Search $q_i$ from $\{l \in L \mid s_{\min}(l) = i\}$ such that $q_i \mid (x_{i_1}, \ldots, x_{n}) = k_i \in K^*$.
3. Return $(q_i, k_i)$ if such $q_i$ exists.
4. Return $(0, \emptyset)$ if $i = 1$.
5. Evaluate \( k_{i-1} = \frac{p_{i-1} - c_{\min}(p_{i-1}) x_{i-1}}{c_{\min}(p_{i-1})} \bigg|_{(x_1,\ldots,x_n) = k_i} \in K. \)\(^7\)

6. Set \( k_{i-1} = (k_{i-1}, k_i) \).

7. Update \( i \leftarrow i - 1 \), and go back to step 2.

Another is the classical elimination procedure with an evidence of conflict.

**Process A.2.**

Input: A pivot sequence \((p_1, \ldots , p_{j-1})\) and a pair \((q_i, k_i) \neq (0, \emptyset)\) which satisfies the output conditions in Process A.1.

Output: A combination \( q_j \in K_{q_i,p_1,\ldots,p_j}^* \) such that \( s_{\min}(q_j) = j. \)\(^8\)

1. Set \( q = q_i. \)

2. For \( h \) from \( i \) to \( j - 1 \), update \( q \leftarrow q - \frac{c_{\min}(q)}{c_{\min}(p_h)} p_h \) if \( h = s_{\min}(q). \)

3. Return \( q_j = q. \)

We can construct a process to find a new pivot combination by combining Processes A.1 and A.2.

**Process A.3.**

Input: Combinations \( l_1, \ldots , l_m \) and a pivot sequence \((p_1, \ldots , p_{j-1})\).

Output: Either 0 or a combination \( p_j \in K_{l_1,\ldots,l_m,p_1,\ldots,p_j}^* \) such that \( s_{\min}(p_j) = j. \)

1. Receive \((q_i, k_i)\) from Process A.1 for the inputs \( L = \{l_1, \ldots , l_m\} \) and \((p_1, \ldots , p_{j-1})\).

2. Return 0 if \( q_i = 0. \)

3. Receive \( q_j \) from Process A.2 for the inputs \((p_i, \ldots , p_{j-1})\) and \((q_i, k_i)\).

4. Return \( p_j = q_j. \)

Process A.3 is essential for finding a pivot combination whose minimum variable is \( x_j \), because we can find out it by Process A.3 if and only if it exists.

**Proposition A.4.** For combinations \( l_1, \ldots , l_m \) and a pivot sequence \((p_1, \ldots , p_{j-1})\), the following statements are equivalent.

(i) Process A.3 outputs \( p_j \in K_{l_1,\ldots,l_m,p_1,\ldots,p_{j-1}}^* \) such that \( s_{\min}(p_j) = j. \)

(ii) There exists a combination \( p_j \in K_{l_1,\ldots,l_m,p_1,\ldots,p_{j-1}}^* \) such that \( s_{\min}(p_j) = j. \)

---

\(^7\)This evaluation is well-defined since \( s_{\min}(p_{i-1}) = i - 1 \) and \( c_{\min}(p_{i-1}) \neq 0. \) The condition (d) follows from

\[ p_{i-1} \bigg|_{(x_1,\ldots,x_n) = (k_{i-1},\ldots,k_n)} = c_{\min}(p_{i-1}) k_{i-1} + (p_{i-1} - c_{\min}(p_{i-1}) x_{i-1}) \bigg|_{(x_1,\ldots,x_n) = (k_{i-1},\ldots,k_n)} = 0. \]

\(^8\)The theory of Gaussian elimination only ensures \( q_j \in K_{q_i,p_1,\ldots,p_{j-1}}^* \) and \( s_{\min}(q_j) \geq j. \) However, updating method of \( q \) in step 2, together with the output conditions (c) and (d) in Process A.1, implies \( q_j \bigg|_{(x_1,\ldots,x_n) = k_i} \in K^*. \) It also implies \( s_{\min}(q_j) = j. \) In fact, if \( s_{\min}(q_j) > j, \)

\[ q_j \bigg|_{(x_1,\ldots,x_n) = k_i} = q_j \bigg|_{(x_{j+1},\ldots,x_n) = (k_{j+1},\ldots,k_n)} = q_j \bigg|_{x_{j+1} = \cdots = x_n = 0} = 0, \]

which is a contradiction. Therefore the output condition in Process A.2 holds.
We call an integer in $D$, step 4, we conclude (i) Algorithm A.6.

Proof. Obviously, (i) implies (ii). Suppose (ii) is true to prove the converse. Then there exist elements $c_1, \ldots, c_m, d_1, \ldots, d_{j-1}$ in $K$ such that

$$p_j = \sum_h c_h l_h + \sum_i d_ip_i.$$  

We have $p_j \mid (x_j, x_{j+1}, \ldots, x_n)=(1,0,0) \in K^*$ since $x_j$ is the minimum variable in $p_j$.

We first consider the situation where we run Process A.1 for the inputs $L = \{l_1, \ldots, l_m\}$ and $(p_1, \ldots, p_{j-1})$: however, we temporally assume that step 3 is skipped and the process ends with the output $(0, \emptyset)$ at step 4 of $i = 1$. Let $k_1, \ldots, k_{j-1}$ be the elements in $K$ which are recursively determined as at step 5, and let $k = (k_1, \ldots, k_{j-1}, 1, 0, \ldots, 0) \in K^n$. Then $p_1(k) = \cdots = p_{j-1}(k) = 0$, and

$$p_j(k) = \sum_h c_h l_h(k) + \sum_i d_ip_i(k) = \sum_h c_h l_h(k).$$

Since $p_j(k) = p_j \mid (x_j, x_{j+1}, \ldots, x_n)=(1,0,0) \in K^*$, this implies $l_h(k) \in K^*$ for some $h$, which means that Process A.1 can find out $q_i$ in step 2 such that $q_i \mid (x_1, \ldots, x_n)=k_i \in K^*$, at least when $i = s_{\min}(l_h)$. Therefore, Process A.1 without the temporal assumption always outputs $(q_i, k_i) \neq (0, \emptyset)$.

We input $L = \{l_1, \ldots, l_m\}$ and $(p_1, \ldots, p_{j-1})$ into Process A.3. At step 1, we receive $(q_i, k_i) \neq (0, \emptyset)$ from Process A.1. Thus step 2 is skipped, and $q_j$ is received from Process A.2 at step 3, which satisfies the condition required in (i). Since $p_j = q_j$ is returned at step 4, we conclude (i) holds.

For a subscript $j$ and a pivot sequence $(p_g) = (p_g)_{1 \leq g \leq h}$ with $i_h < j$, we define

$$D(p_g, j) := [j - 1] \setminus \{i_1, \ldots, i_h\}.$$  

We call an integer in $D(p_g, j)$ a deficient subscript, and a variable $x_i$ with $i \in D(p_g, j)$ a deficient variable.

We need to modify Process A.3 for practical use.

**Process A.5.**

Input: Combinations $l_1, \ldots, l_m$, a subscript $j$, and a pivot sequence $(p_g)_{1 \leq g \leq h}$ with $i_h < j$.

Output: Either 0 or a combination $p_j \in K^*_{l_1, \ldots, l_m, p_{a_1}, \ldots, p_{a_h}}$ with $s_{\min}(p_j) \in D(p_g, j) \cup \{j\}$.

1. Change the variable order by moving the deficient variables backward.
2. Prepare the pivot sequence $(p'_{j-1}, \ldots, p'_{j-1-|D(p_g, j)|})$ for the new variable order.
3. Receive $p'_{j-1-|D(p_g, j)|}$ from Process A.3 for the inputs $l_1, \ldots, l_m$ and $(p'_{j-1}, \ldots, p'_{j-1-|D(p_g, j)|})$.
4. Undo the variable order by putting the deficient variables back to their original places.
5. Return $p_j = p'_{j-1-|D(p_g, j)|}$.

We are in a position to state Algorithm A.6 for a fast Gaussian forward elimination.

**Algorithm A.6.**

Input: Combinations $L = \{l_1, \ldots, l_m\}$.
Output: A pivot sequence \((p_i)\).

1. Create subsets \(L_i = \{l \in L | s_{\min}(l) = i\} \ (i = 1, \ldots, n)\).

2. Set \(j = 0\) and \((p_i) = \emptyset\).

3. Execute the following loop process to make a pivot sequence \((p_i)\):
   
   (i) Update \(j \leftarrow j + 1\) if \(j < n\); otherwise break.
   
   (ii) If \(L_j \neq \emptyset\), append a combination in \(L_i\) to \((p_i)\) and go back to (i).
   
   (iii) Receive \(p_j\) from Process A.5 for the inputs \(L_1 \cup \cdots \cup L_{j-1}\) and \((p_i)\).
   
   (iv) If \(p_j = 0\), go back to (i).
   
   (v) Append \(p_j\) to \((p_i)\), and back to (i).

4. Return \((p_i)\).

The pivot sequence \((p_i)\) outputted by Algorithm A.6 is a row echelon matrix under the order \(x_1 < \cdots < x_n\) thanks to Proposition A.4 (see the footnote in (v) of step 3 for details).

**Remark A.7.** Process A.1 is influenced by the unit propagation (UP) in the algorithm to solve the Boolean satisfiability (SAT) problem (see, e.g., [3, Chapter 1]). SAT is the first problem that was proved to be NP-complete, which means that all NP-problems are at most as difficult as SAT. UP is a technique to determine an assignment value for the variable we watch while searching a conflict combination (or a conflict clause in SAT terminology).

Process A.2 is inspired by the conflict-driven clause learning (CDCL) proposed in [2, 24, 25] (see also [3, Chapter 5]). CDCL enable us to find (or learn) a new pivot combination from the conflict evidence found by UP.

The performance of UP tends to increase when combinations have good structures for finding conflict combinations under a good variable order: i.e., not too few number of combinations, high frequency of small size combinations, bias of occurrences of variables, and so on. We have seen in Table 7 that the runtimes of MJPO and EDS are much better than those of KNT, which seems to be due to the difference in numbers of relations (or combinations).

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The loop process ensures \(s_{\min}(p_j) = j\). To show this, we may prove \(s_{\min}(p_j) \notin D_{(p_i), j}\) by the output condition in Process A.5. Suppose \(s_{\min}(p_j) \in D_{(p_i), j}\) and set \(j' = s_{\min}(p_j) < j\). Then, on the \(j'\)-round in the loop process, Process A.5 at (iii) must return a non-zero combination by Proposition A.4 and the existence of \(p_j\), where note that Process A.5 is essentially Process A.3. This means a combination \(p_{j'}\) satisfying \(s_{\min}(p_{j'}) = j'\) must be appended to \((p_i)\) at (v) on the \(j'\)-round, which contradicts \(j' = s_{\min}(p_j) \in D_{(p_i), j}\).
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