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Some Multi-Set Inclusions Associated with Shuffle Convolutions and Multiple Zeta Values

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Abstract. We outline a new technique for proving certain shuffle convolution formulæ. As an application, we give a new combinatorial proof of the formula $\zeta(\{3,1\}^n) = 2\pi^{4n}/(4n+2)!$ for multiple zeta values.

1 Shuffles

As in [5, 6, 13] let X be a finite set and let X^* denote the free monoid generated by X. We regard X as an alphabet, and the elements of X^* as words formed by concatenating any finite number of letters (repetitions permitted) from X. By linearly extending the concatenation product to the set $\mathbf{Q}\langle X\rangle$ of rational linear combinations of elements of X^*, we obtain a non-commutative polynomial ring with multiplicative identity 1 denoting the empty word.

The shuffle product may be defined on words by the recursion

$$\begin{cases} \forall w \in X^*, & 1 \sqcup\!\sqcup\, w = w \sqcup\!\sqcup\, 1 = w, \\ \forall a, b \in X, \quad \forall u, v \in X^*, & au \sqcup\!\sqcup\, bv = a(u \sqcup\!\sqcup\, bv) + b(au \sqcup\!\sqcup\, v), \end{cases}$$

and then extended linearly to $\mathbf{Q}\langle X\rangle$. One checks that the shuffle product so defined is associative and commutative, and thus $\mathbf{Q}\langle X\rangle$ equipped with the shuffle product becomes a commutative $\mathbf{Q}$-algebra, denoted $\mathrm{Sh}_{\mathbf{Q}}[X]$. Radford [14] has shown that $\mathrm{Sh}_{\mathbf{Q}}[X]$ is isomorphic to the polynomial algebra $\mathbf{Q}[L]$ obtained by adjoining the transcendence basis L of Lyndon words to the field $\mathbf{Q}$ of rational numbers. The study of shuffles was initiated by Chen [8, 9] and subsequently formalized by Ree [15]. Interest in shuffles has revived due to the intimate connection with multiple zeta values [1, 3, 4, 5, 7, 11, 12, 16] and multiple polylogarithms [2, 6, 10, 17], which we briefly indicate here. For details, we refer the reader to [5], and the survey paper [6].

For $|x| \le 1$ and positive integers $s_1, \dots, s_k$, the nested sum of depth k defined by

$$\zeta_x(s_1, \dots, s_k) := \sum_{n_1 > \cdots > n_k > 0} x^{n_1} \prod_{j=1}^{k} n_j^{-s_j} \tag{1}$$

is an instance of a multiple polylogarithm [2, 6, 10, 17]. The subscript x is commonly dropped when $x = 1$, in which case (1) is called a multiple zeta value. Thus,

$$\zeta(s_1, \dots, s_k) := \sum_{n_1 > \cdots > n_k > 0} \prod_{j=1}^{k} n_j^{-s_j}. \tag{2}$$

It turns out that for $0 < x \le 1$, the multiple polylogarithm (1) admits the simplex integral representation [6, 18]

$$\zeta_x(s_1, \dots, s_k) = \int \prod_{j=1}^{k} \left(\prod_{r=1}^{s_j - 1} \frac{dt_r^{(j)}}{t_r^{(j)}} \right) \frac{dt_{s_j}^{(j)}}{1 - t_{s_j}^{(j)}},$$

where the integral is over the simplex

$$x > t_1^{(1)} > \cdots > t_{s_1}^{(1)} > \cdots > t_1^{(k)} > \cdots > t_{s_k}^{(k)} > 0,$$

and is abbreviated [1, 2, 3, 5] by

$$\zeta_x(s_1, \dots, s_k) = \int_0^x \prod_{j=1}^{k} A^{s_j - 1} B, \qquad A = dt/t, \qquad B = dt/(1-t). \tag{3}$$

The definition of the shuffle product is motivated by the elementary fact that the product of two simplex integrals consists of a sum of simplex integerals over all possible interlacings of the respective variables of integration. Explicitly, if

$$\int_y^x \prod_{j=1}^{n} a_j := \int_{x > t_1 > \cdots > t_n > y} \prod_{j=1}^{n} f_j(t_j)\, dt_j, \qquad a_j := f_j(t_j)\, dt_j,$$

then [2, 5, 6]

$$\left(\int_y^x \prod_{j=1}^{m} a_j\right)\left(\int_y^x \prod_{j=m+1}^{m+n} a_j\right) = \int_y^x \left[\left(\prod_{j=1}^{m} a_j\right) ш \left(\prod_{j=m+1}^{m+n} a_j\right)\right].$$

In what follows, if X is an alphabet and $u, v \in X^*$, we'll denote by $\{u ш v\}$ the multi-set of words appearing (with multiplicity) in the expansion of $u ш v$. For example, suppose $X = \{a, b\}$. Since $ab ш ab = 4aabb + 2abab$, we have

$$\{ab ш ab\} = \{abab, abab, aabb, aabb, aabb, aabb\},$$

which, as a multi-set, *properly* contains $\{abab, aabb\}$. The following result states that the multi-sets formed by shuffling certain pairs of words defined periodically comprise two symmetric chains of inclusions. The largest member of the chain is attained when the words in the pair being shuffled are of equal length.

Theorem 1 *Let r be a positive integer, let X be an alphabet, and let $a_1, a_2, \ldots \in X$ be such that $a_{r+m} = a_m$ for all positive integers m. Fix a positive integer n, put $S_0 = S_{2n} = \{a_1 a_2 \cdots a_{2nr}\}$, and define multi-sets $S_k = \{a_1 a_2 \cdots a_{kr} ш a_1 a_2 \cdots a_{(2n-k)r}\}$, for integer k satisfying $1 \le k \le 2n-1$. Then $S_{k-1} \subseteq S_k$ for $k = 1, 2, \ldots, n$, and $S_{k+1} \subseteq S_k$ for $k = n, n+1, \ldots, 2n-1$.*

2 Consequences

Interestingly, Theorem 1 can be used to give a very short proof of a non-trivial shuffle convolution formula which has been shown [3] to imply the closed-form evaluation

$$\zeta(\{3,1\}^n) := \zeta(\underbrace{3, 1, \ldots, 3, 1}_{2n \text{ arguments}}) = \frac{2\pi^{4n}}{(4n+2)!}, \qquad 1 \le n \in \mathbf{Z}, \tag{4}$$

for the multiple zeta function (2). The formula (4) was originally conjectured by Zagier [18] on the basis of numerical evidence. It was subsequently proved by Broadhurst, in collaboration with Borwein and Bradley. A modification of Broadhurst's proof due to Zagier appears in [2]: see Theorem 11.1 and Corollary 2 there. Subsequently, a combinatorial proof was found [3] based on the following result, of which we give an independent derivation here.

Corollary 1 (Corollary 1 of [3]) *Let n be a positive integer, and let $\{a, b\}$ be an alphabet. Then*

$$\sum_{k=0}^{2n} (-1)^{n+k} [(ab)^k ш (ab)^{2n-k}] = (4a^2b^2)^n. \tag{5}$$

Proof. In Theorem 1, let $X = \{a, b\}$ and $r = 2$. In view of the multi-set inclusions indicated by Theorem 1, there must be

$$\sum_{k=0}^{2n}(-1)^{n+k}|S_k| = \sum_{k=0}^{2n}(-1)^{n+k}\binom{4n}{2k} = 4^n$$

words on each side of (5), counting multiplicity. Furthermore, the word $(a^2b^2)^n$ occurs 4^n times in S_n, since each a and each b can take two positions. Since $(a^2b^2)^n$ cannot occur in S_k for $k \neq n$, (5) follows immediately. □

Corollary 2 (Corollary 2 of [2], Theorem 1 of [3]) *The formula* (4) *holds; i.e. if n is a positive integer, then*

$$\zeta(\{3,1\}^n) = \frac{2\pi^{4n}}{(4n+2)!}.$$

Proof. The stated formula follows from (5), the well-known fact [1, 11] that $\zeta(\{2\}^n) = \pi^{2n}/(2n+1)!$, and the simplex integral representation (3) for multiple zeta values. See [3] for details. □

Cyclic extensions of (4) beyond those in [3] are given in [5]. Differential equations are exploited in [4] to provide closed-form evaluations for additional multiple zeta values and nested alternating series with periodic argument lists of arbitrary depth. Other shuffle convolution formulæ can be established in a manner similar to our proof of Corollary 1. For example, if $\{a, b\}$ is an alphabet and n is a positive integer, then

$$2\sum_{k=0}^{2n}(-1)^{n+k}[(ab)^k \sqcup\!\sqcup (ba)^{2n-k}] = (4abba)^n + (4baab)^n.$$

As a final observation, we note that Theorem 1 implies the unimodality of the binomial coefficients. More specifically, we have the following:

Corollary 3 *Let n and r be positive integers. The finite sequence $b_0, b_1, \ldots, b_{2n}$ defined by*

$$b_k = \binom{2nr}{kr}, \qquad 0 \le k \le 2n,$$

is unimodal.

Proof. Note that the cardinality of the multi-set S_k in Theorem 1 is equal to b_k. □

3 Proving the Multi-Set Inclusions

Proof of Theorem 1. Since the shuffle product is commutative, $S_k = S_{2n-k}$ for $0 \leq k \leq 2n$, and so it suffices to prove that $S_{k-1} \subseteq S_k$ for $k = 1, 2, \ldots, n$. To help clarify the formation of words in the multi-sets S_k, write

$$S_k = \{a_1 \cdots a_{kr} ⧢ A_1 \cdots A_{(2n-k)r}\}, \qquad 1 \leq k \leq n,$$

where $A_j = a_j$ for each positive integer j. We have $S_1 = \{a_1 \cdots a_r ⧢ A_1 \cdots A_{(2n-1)r}\}$ and $S_0 = \{a_1 a_2 \cdots a_{2nr}\}$. Since periodicity implies

$$a_1 \cdots a_{2nr} = a_1 \cdots a_r A_{r+1} \cdots A_{2nr} = a_1 \cdots a_r A_1 \cdots A_{(2n-1)r} \in S_1,$$

it follows that $S_0 \subseteq S_1$. Therefore, we may assume henceforth that $2 \leq k \leq n$.

Let $w \in S_{k-1} = \{a_1 \cdots a_{(k-1)r} ⧢ A_1 \cdots A_{(2n-k+1)r}\}$. It suffices to show that the multiplicity of w in S_k is at least as large as the multiplicity of w in S_{k-1}. If a_1 follows A_r in w, then

$$w \in A_1 \cdots A_r \{a_1 \cdots a_{(k-1)r} ⧢ A_{r+1} \cdots A_{(2n-k+1)r}\}. \tag{6}$$

It is clear that no matter how many times w occurs in the multi-set (6), w must occur the same number of times in the equivalent multi-set

$$a_1 \cdots a_r \{a_{r+1} \cdots a_{kr} ⧢ A_1 \cdots A_{(2n-k)r}\} \subseteq S_k.$$

It follows that the multiplicity of w in S_k is no less than the multiplicity of w in S_{k-1} in this case. Therefore, we may assume a_1 precedes A_r in w.

Proceeding inductively, suppose that p is a positive integer for which a_p precedes A_{r+p-1} in w. Note that if also a_{p+1} follows A_{r+p}, then w must lie in the multi-set

$$\{A_1 \cdots A_{r+p-2} ⧢ a_1 \cdots a_p\} A_{r+p-1} A_{r+p} \{a_{p+1} \cdots a_{(k-1)r} ⧢ A_{r+p+1} \cdots A_{(2n-k+1)r}\}. \tag{7}$$

But, it is clear that no matter how many times w occurs in the multi-set (7), w must occur the same number of times in the equivalent multi-set

$$\{a_1 \cdots a_{r+p-2} ⧢ A_1 \cdots A_p\} a_{r+p-1} a_{r+p} \{a_{r+p+1} \cdots a_{kr} ⧢ A_{p+1} \cdots A_{(2n-k)r}\} \subseteq S_k.$$

By induction, we may therefore assume that $a_{(k-1)r}$ precedes A_{kr-1} in w, in which case w must lie in the multi-set

$$\{a_1 \cdots a_{(k-1)r} ⧢ A_1 \cdots A_{kr-2}\} A_{kr-1} \cdots A_{(2n-k+1)r}. \tag{8}$$

Again, no matter how many times w occurs in the multi-set (8), w must occur the same number of times in the equivalent multi-set

$$\begin{aligned} &\{A_1 \cdots A_{(k-1)r} ⧢ a_1 \cdots a_{kr-2}\} a_{kr-1} a_{kr} A_{kr+1} \cdots A_{(2n-k+1)r} \\ = &\{A_1 \cdots A_{(k-1)r} ⧢ a_1 \cdots a_{kr-2}\} a_{kr-1} a_{kr} A_{(k-1)r+1} \cdots A_{(2n-k)r} \\ \subseteq &S_k, \end{aligned}$$

and the proof is complete. $\square$

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