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 the alphabet \( X \). By linearly extending the concatenation product to the set \( \mathbb{Q}_\{X\} \) of rational linear combinations of elements of \( X^* \), we obtain a non-commutative polynomial ring with the elements of \( X \) being indeterminates and with multiplicative identity \( 1 \) denoting the empty word.
The shuffle product may be defined on words by the recursion
\[
\begin{align*}
\forall w \in X^*, & \quad 1 \shuffle w = w \shuffle 1 = w, \\
\forall a, b \in X, \forall u, v \in X^*, & \quad au \shuffle bv = a(u \shuffle bv) + b(au \shuffle v),
\end{align*}
\]
and then extended linearly to \( Q(X) \). One checks that the shuffle product so defined is associative and commutative, and thus \( Q(X) \) equipped with the shuffle product becomes a commutative \( Q \)-algebra, denoted \( \text{Sh}_Q[X] \). Radford [14] has shown that \( \text{Sh}_Q[X] \) is isomorphic to the polynomial algebra \( Q[L] \) obtained by adjoining the transcendence basis \( L \) of Lyndon words to the field \( Q \) 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].

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

**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 \( a_{r+k} = a_k \) for all positive integers \( k \). Fix a positive integer \( n \), and define multi-sets
\[
S_k = \{a_1a_2\cdots a_ka_1a_2\cdots a_{(2n-k)r}\}, \quad 0 \leq k \leq 2n.
\]
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

Before proving Theorem 1, we make some observations. First, observe that Theorem 1 generalizes the unimodality of the binomial coefficients. More specifically, we have the following:

**Corollary 1** Let \( n \) and \( r \) be positive integers. The finite sequence \( b_0, b_1, \ldots, b_{2n} \) defined by
\[
b_k = \binom{2nr}{kr}, \quad 0 \leq k \leq 2n,
\]
is unimodal.

**Proof.** Note that the cardinality of the multi-set \( S_k \) in Theorem 1 is equal to \( b_k \). \( \square \)
More interestingly, Theorem 1 implies a non-trivial shuffle convolution formula which has been shown [3] to imply the formula

$$\zeta(\{3,1\}^n) := \zeta(3,1,\ldots,3,1) = \frac{2\pi^{4n}}{(4n + 2)!}, \quad 0 \leq n \in \mathbb{Z},$$

(1)

for the multiple zeta function defined by

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

**Corollary 2** Let \(n\) be a positive integer, and let \(\{a,b\}\) be an alphabet. Then

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

(2)

**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

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

terms on each side of (2), 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 \(k \neq n\), (2) follows immediately. \(\square\)

**Corollary 3** The formula (1) 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 (2) and the iterated integral representation for multiple zeta values. See [3] for details. \(\square\)

### 3 Proving the Multi-Set Inclusions

**Proof of Theorem 1.** Since \(S_k = S_{2n-k}\), it suffices to prove that \(S_{k-1} \subseteq S_k\) for \(k = 1, 2, \ldots, n\). We shall first consider the case when \(k = 1\). Observe that

\(S_1 = \{a_1 \cdots a_r \cup a_1 \cdots a_{(2n-1)r}\}\)

and that \(S_0 = \{a_1 a_2 \cdots a_{2nr}\}\). 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 $S_0 \subseteq S_1$, and so we may assume henceforth that $2 \leq k \leq n$.

To help clarify the formation of words in the multi-sets $S_k$, for $0 \leq k \leq n$, let

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

where $A_j = a_j$ for each positive integer $j$. Now consider a word

$$w \in S_{k-1} = \{a_1 \cdots a_{(k-1)r} \sqcup A_1 \cdots A_{(2n-k+1)r}\}.$$ 

If $a_1$ follows $A_r$ in $w$, then

$$w = A_1 \cdots A_r \{a_1 \cdots a_{(k-1)r} \sqcup A_{r+1} \cdots A_{(2n-k+1)r}\}$$

$$= a_1 \cdots a_r \{a_{r+1} \cdots a_{kr} \sqcup A_1 \cdots A_{(2n-k)r}\}$$

$$\subseteq S_k.$$

Since we could conceivably have made a different choice in replacing certain of the $A_j$ by $a_j$, 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 $w$. If, in addition, $a_2$ follows $A_{r+1}$ in $w$, then

$$w = \{A_1 \cdots A_{r-1} \sqcup a_1\} A_r A_{r+1} \{a_2 \cdots a_{(k-1)r} \sqcup A_{r+2} \cdots A_{(2n-k+1)r}\}$$

$$= \{a_1 \cdots a_{r-1} \sqcup A_1\} a_r a_{r+1} \{a_{r+2} \cdots a_{kr} \sqcup A_2 \cdots A_{(2n-k)r}\}$$

$$\subseteq S_k.$$

Therefore, we may assume $a_2$ precedes $A_{r+1}$ in $w$.

In general, given that $a_p$ precedes $A_{r+p-1}$ in $w$, we note that if $a_{p+1}$ follows $A_{r+p}$, then $w$ lies in the multi-set

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

$$= \{a_1 \cdots a_{r+p-2} \sqcup A_1 \cdots A_p\} a_{r+p-1} a_{r+p} \{a_{r+p+1} \cdots a_{kr} \sqcup A_{p+1} \cdots A_{(2n-k)r}\}$$

$$\subseteq S_k.$$

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

$$\{a_1 \cdots a_{(k-1)r} \sqcup A_1 \cdots A_{kr-2}\} A_{kr-1} A_{kr} \cdots A_{(2n-k+1)r}$$

$$= \{A_1 \cdots A_{(k-1)r} \sqcup a_1 \cdots a_{kr-2}\} a_{kr-1} a_{kr} A_{kr+1} \cdots A_{(2n-k+1)r}$$

$$= \{A_1 \cdots A_{(k-1)r} \sqcup a_1 \cdots a_{kr-2}\} a_{kr-1} a_{kr} A_{(k-1)r+1} \cdots A_{(2n-k)r}$$

$$\subseteq S_k.$$ 

□

Other shuffle convolution formulæ can be established in a similar manner. For example, if $\{a, b\}$ is an alphabet and $n$ is a positive integer, then

$$2 \sum_{k=0}^{2n} (-1)^{n+k} [(ab)^k \sqcup (ba)^{2n-k}] = (Aabba)^n + (Abaab)^n.$$
References


