Application of Unspecified Sequences in Symbolic Summation

Manuel Kauers*
RISC-Linz
Johannes Kepler Universität
A-4040 Linz, Austria
mkauers@risc.uni-linz.ac.at

Carsten Schneider*
RISC-Linz
Johannes Kepler Universität
A-4040 Linz, Austria
cschneid@risc.uni-linz.ac.at

ABSTRACT
We consider symbolic sums which contain subexpressions that represent unspecified sequences. Existing symbolic summation technology is extended to sums of this kind. We show how this can be applied in the systematic search for general summation identities. Both, results about the non-existence of identities of a certain form, and examples of general families of identities which we have discovered automatically are included in the paper.

Categories and Subject Descriptors
I.1.2 [**Computing Methodologies**]: Symbolic and Algebraic Manipulation—*Algorithms*; G.2.1 [**Discrete Mathematics**]: Combinatorics—*Recurrences and difference equations*

General Terms
Algorithms

Keywords
Symbolic Summation, Difference Fields

1. INTRODUCTION
The focus of this paper is on summation identities involving expressions like X_k that stand for *unspecified sequences*. Such summation identities remain true for every particular sequence f_k in place of the symbol X_k. A simple example for such an identity is

$$\sum_{k=0}^{n}(X_{k+1}-1)\prod_{i=0}^{k}X_i=\prod_{k=0}^{n+1}X_k-X_0. \tag{1}$$

*Both authors were supported by the Austrian science foundation FWF, grants P16613-N12 and F1305.

If particular rational functions are substituted for X_k in this identity, we obtain precisely the indefinite hypergeometric summation identities that are found by Gosper's algorithm [5, 12]. We may say that Gosper's algorithm precisely solves the task of writing a given hypergeometric term in the form $(X_{k+1}-1)\prod_{i=0}^{k}X_i$ for a specific rational function, or it proves that this is impossible.

In the present paper, we mainly study definite summation identities involving unspecified sequences. A sum is called definite if the summand depends not only on the summation index k but also on the summation bound n. A simple example is

$$\sum_{k=0}^{n}X_{n+k}=X_0+\sum_{k=0}^{n-1}(X_{2k+1}+X_{2k+2}-X_k)$$

Again, the identity holds for every sequence in place of the symbol X_k. The interest in identities of this type was not so much raised by examples arising from practice. The consideration of summation identities involving unspecified sequences X_k is rather motivated because the presence of X_k in summation identities reveals some structural information about summation in general and summation algorithms in particular. Usage of unspecified sequences makes it possible to search for (families of) "nice" summation identities in a more systematic way. For instance, criteria can be automatically derived which a sequence f_k in place of X_k must fulfill such that a closed form can be found (Section 4).

An earlier paper of ours [8] contains an algorithm for indefinite summation with unspecified sequences. In Section 2 we discuss how this algorithm can be extended to definite summation via the creative telescoping method [22]. This algorithm was implemented and incorporated into the second author's summation package Sigma [17]. With this implementation, we then searched for general definite summation identities involving unspecified sequences. It turned out that only very few general identities exist. An explanation for this phenomenon is provided in Section 3, where we show that a certain class of definite sums does not admit creative telescoping recurrences at all.

This negative result suggests that the search for nontrivial general summation identities has to be focused on more complicated expressions, such as nested sum expressions. Even in this enlarged domain, general definite sums which admit simplification are rare. Some which we have found by experimenting are presented in Section 4.

2. SUMMATION IN DIFFERENCE FIELDS

2.1 PLDEs and Summation

A fundamental role in summation algorithms is played by *parameterized linear difference equations* (PLDEs): Given certain sequences $a_0,\dots,a_m$ and $f_0,\dots,f_r\colon\mathbb{N}\to\mathbb{K}$, where $\mathbb{K}$ is a field, the goal is to find a sequence g and constants $c_0,\dots,c_r$ such that

$$a_0g+a_1Eg+\cdots+a_mE^mg=c_0f_0+\cdots+c_rf_r,\qquad(2)$$

where E denotes the shift operator $(Ef)_k:=f_{k+1}$.

Indefinite summation provides the most special situation. Here, we seek a closed form expression for a sum $\sum_{k=0}^n f_k$ with f_k independent of n. If g is a solution of (2) with $a_0=-1$, $a_1=1$, $f_0=f$ (telescoping equation), then we have $\sum_{k=0}^n f_k=g_{n+1}-g_0$.

Less straightforward are definite sums. These are sums of the form $S_n=\sum_{k=0}^n f_{n,k}$, where $f_{n,k}$ may depend on both, the summation index k and the bound n. For such sums, telescoping normally fails. Therefore, we proceed in two steps: First, we compute a recurrence equation for the sum by means of *creative telescoping* [22], and in a second step we solve that recurrence. In creative telescoping, we consider k as the independent variable and n as constant, and we solve

$$Eg-g=c_0f_0+c_1f_1+\cdots+c_rf_r\qquad(3)$$

with $f_i=f_{n+i,k}$ (another special case of (2)). Once a solution $(c_0,\dots,c_r,g)$ is known, we can derive a recurrence for the original sum S_n by summing the equation over k. This recurrence is of the form

$$a_0g+a_1Eg+\cdots+a_rE^rg=f$$

(another special case of (2)) for certain $a_0,\dots,a_r,f$ which originate from $c_0,\dots,c_r$, and g. Now n is considered as independent variable, and k is no longer present. Solving this equation for g delivers a closed form for the definite sum S_n.

This general summation strategy is explained in detail for hypergeometric summation in [14]. The same technique is applicable for more general expressions.

Example 1. Consider the definite sum $S_n=\sum_{k=0}^n f_{n,k}$ with $f_{n,k}=kX_{n+k}$. Applying creative telescoping for $r=2$, we have to find constants c_0,c_1,c_2 and some $g_{n,k}$ such that

$$\begin{aligned}g_{n,k+1}-g_{n,k}&=c_0f_{n,k}+c_1f_{n+1,k}+c_2f_{n+2,k}\\&=c_0kX_{n+k}+c_1kX_{n+k+1}+c_2kX_{n+k+2}.\end{aligned}$$

It is easily checked that a solution is given by $(c_0,c_1,c_2)=(1,-2,1,(k-1)X_{n+k+1}-kX_{n+k})$. Summing the equation over k from 0 to n and compensating missing terms gives the recurrence

$$S_n-2S_{n+1}+S_{n+2}=f_n$$

with

$$\begin{aligned}f_n&=-X_{n+1}+(n+1)X_{2n+1}\\&\quad+(n+2)X_{2n+2}-(n+1)X_{2n+3}-(n+2)X_{2n+4}.\end{aligned}$$

Next, we have to solve this recurrence. The homogeneous equation obviously has the solutions 1 and n, and it turns out that the inhomogeneous equation has the particular solution $-\sum_{k=0}^n\sum_{i=0}^k f_{i-2}$. Comparison of two initial values reveals the representation

$$S_n=-\sum_{k=0}^n\sum_{i=0}^k f_{i-2}.\qquad(4)$$

This can be simplified further, as we will see below (Example 3).

This summation process can be carried out computationally in the general setting of *difference fields* [17]. A difference field is a pair $(\mathbb{F},\sigma)$ where $\sigma\colon\mathbb{F}\to\mathbb{F}$ is a field automorphism. The elements of a difference field are understood as formalizations of sequences, and the automorphism σ should act on the field elements like the shift operator $(Ef)_k=f_{k+1}$ acts on the corresponding sequences. The elements $c\in\mathbb{F}$ with $\sigma(c)=c$ form a subfield $\mathbb{K}$ of $\mathbb{F}$, called the *field of constants.* In the language of difference fields, the problem of solving parameterized linear difference equation reads as follows:

GIVEN: A difference field $(\mathbb{F},\sigma)$ with constant field $\mathbb{K}$ and elements $a_0,\dots,a_m\in\mathbb{F}$ and $f_0,\dots,f_r\in\mathbb{F}$

FIND: All tuples $(c_0,\dots,c_r,g)\in\mathbb{K}^{r+1}\times\mathbb{F}$ such that

$$a_0g+a_1\sigma(g)+\cdots+a_m\sigma^m(g)=c_0f_0+\cdots+c_rf_r.\qquad(5)$$

It is easy to check that all the solutions $(c_0,\dots,c_r,g)$ of a parameterized linear difference equation form a vector space over $\mathbb{K}$, and we want to compute a basis of this vector space. Of course, it might be that there do not exist solutions in the given field $\mathbb{F}$. In this case, it is of interest to construct a bigger field where there exists a "nice" solution. This will be used in Section 4 for deriving criteria on the X_k that make a given sum summable in closed form.

Algorithms for solving PLDEs are available for several types of difference fields $(\mathbb{F},\sigma)$. For the simplest case of a constant field, i.e., $\mathbb{F}=\mathbb{K}$, the solution of a PLDE is immediate by linear algebra. In the remainder of this section, we will outline solution algorithms for free difference fields and $\Pi\Sigma$-extensions. Difference fields constructed from free difference fields by $\Pi\Sigma$-extensions are the appropriate fields for the summation problems we want to consider later in this paper.

2.2 Solving PLDEs in free difference fields

All difference fields which we consider in this paper are constructed as (iterated) difference field extensions over some constant field $\mathbb{K}$. A difference field extension of some difference field $(\mathbb{G},\sigma)$ is a difference field which is obtained by adjoining one or more transcendental elements $t,t',t'',\dots$ to $\mathbb{G}$ and extending the definition of the shift σ to this extended field $\mathbb{G}(t,t',t'',\dots)$.

As the *free* difference field extension of a difference field $(\mathbb{F},\sigma)$ (by a *difference variable* x), we define the field

$$\mathbb{F}\langle x\rangle:=\mathbb{F}(\dots,x_{-2},x_{-1},x_0,x_1,x_2,\dots).$$

The shift σ is extended from $\mathbb{F}$ to $\mathbb{F}\langle x\rangle$ by the definition $\sigma(x_i) := x_{i+1}$ ($i \in \mathbb{Z}$). We understand here that the set $\{ x_i : i \in \mathbb{Z}\}$ is algebraically independent over $\mathbb{F}$. A difference variable x is an appropriate algebraic representation of an unspecified sequence [7].

Difference fields which are constructed by iterated free extensions of the constant field $\mathbb{K}$, e.g., $\mathbb{F} = \mathbb{K}\langle x\rangle\langle y\rangle$, are called *free difference fields*. Free difference fields are very easy to deal with computationally, because for each $f \in \mathbb{F}\langle x\rangle \setminus \mathbb{F}$, the forward and backward shift $\sigma(f)$ and $\sigma^{-1}(f)$ both must contain some variable x_i which does not appear in f itself. This makes it possible to devise a solving algorithm based on simple cancellation considerations. We have already described such an algorithm in an earlier paper [8], and abstain here from repeating its details.

2.3 Solving PLDEs in $\Pi\Sigma^*$-Extensions

In his seminal paper, Karr [6] has introduced the notion of $\Pi\Sigma$-fields for representing nested sum and product expressions in difference fields. A simplified version of these fields are the $\Pi\Sigma^*$-fields [15]. These are difference fields which are obtained from a constant field $\mathbb{K}$ by adjoining formal sums or products. To be precise, $(\mathbb{G}(t), \sigma)$ is called a $\Pi\Sigma^*$-extension of a difference field $(\mathbb{G}, \sigma)$, if both difference fields share the same field of constants, t is transcendental over $\mathbb{G}$, and $\sigma(t) = t+r$ for some $r \in \mathbb{G}$ (then t represents a sum) or $\sigma(t) = r \cdot t$ for some $r \in \mathbb{G}$ (then t represents a product). A $\Pi\Sigma^*$-field is a difference field $(\mathbb{K}(t_1, \ldots, t_e), \sigma)$ which is obtained from a constant field $\mathbb{K}$ by repeated $\Pi\Sigma^*$-extensions. In short, we say that $(\mathbb{G}(t_1, \ldots, t_e), \sigma)$ is a (nested) $\Pi\Sigma^*$-extension of $(\mathbb{G}, \sigma)$ if all the t_i are $\Pi\Sigma^*$-extensions.

It is known how to solve PLDEs in $\Pi\Sigma^*$-fields [20]. Here, we are interested in difference fields which are obtained by building a tower of $\Pi\Sigma^*$-extensions on top of a free difference field.

Example 2. For representing the sum from Example 1 above, we choose the difference field $(\mathbb{Q}\langle x\rangle(k), \sigma)$, where $(\mathbb{Q}\langle x\rangle, \sigma)$ is a free difference field and $\sigma(k) = k + 1$. In this field, $f_{n+i,k+j}$ ($i, j \in \mathbb{Z}$) is represented by $(k + j)x_{i+j}$. The creative telescoping equation admits a solution in the same field (compare Example 1). The recurrence obtained for the whole sum, however, requires besides n and X_n the representation of X_{2n} and X_{2n+1}. We take $(\mathbb{Q}\langle x\rangle\langle y\rangle\langle z\rangle(n), \sigma)$ with x, y, z free (representing X_n, X_{2n}, and X_{2n+1}, respectively) and $\sigma(n) = n + 1$. The solutions 1 and n of the homogeneous equation can be represented in the same field, but for representing the particular solution, we have to change to the bigger field $(\mathbb{Q}\langle x\rangle\langle y\rangle\langle z\rangle(n)(t_1)(t_2), \sigma)$, which is a $\Pi\Sigma^*$-extension of the original one [1, 15]. Here $\sigma(t_1) = t_1+\sigma^{-1}(f)$ and $\sigma(t_2) = t_2 + \sigma(t_1)$, where

$$f = -(-x_1 + (n+1)z_0 + (n+2)y_1 - (n+1)z_1 - (n+2)y_2).$$

The particular solution is then t_2 (compare again Example 1).

Subsequently, let $\mathbb{K}$ be a field of constants, $\mathbb{G}$ be obtained from $\mathbb{K}$ by extension of zero or more free difference variables, and $\mathbb{F}$ be obtained from $\mathbb{G}$ by zero or more $\Pi\Sigma^*$-extensions, say $\mathbb{F} = \mathbb{G}(t_1, \ldots, t_e)$. In such a field, PLDEs can be solved very much as in $\Pi\Sigma^*$ fields. Let $\mathbb{F}(t)$ be a $\Pi\Sigma^*$-extension of $\mathbb{F}$. We outline a method which reduces the problem of solving a PLDE in $\mathbb{F}(t)$ to solving several PLDEs in $\mathbb{F}$. Only a rough overview is given, some remarks on technical details and pointers to literature are given in the end of the section.

Reduction I (denominator bounding). Compute a polynomial $d \in \mathbb{F}[t]^*$ such that for all $c_i \in \mathbb{K}$ and $g \in \mathbb{F}(t)$ with (5) we have $dg \in \mathbb{F}[t]$. Then it follows that

$$\frac{a_0}{d} g' + \cdots + \frac{a_m}{\sigma^m(d)} \sigma^m(g') = c_0 f_0 + \cdots + c_r f_r \qquad (6)$$

for $g' \in \mathbb{F}[t]$ if and only if (5) with $g = g'/d$.

Reduction II (degree bounding). Given such a denominator bound, it suffices to look only for $c_i \in \mathbb{K}$ and polynomial solutions $g \in \mathbb{F}[t]$ with (5). Next, we compute a degree bound $b \in \mathbb{N}_0$ for these polynomial solutions.

Reduction III (polynomial degree reduction). Given such a degree bound one looks for $c_i \in \mathbb{K}$ and $g_i \in \mathbb{F}$ such that (5) holds for $g = \sum_{i=0}^{b} g_i t^i$. This can be achieved as follows. First derive the possible leading coefficients g_b by solving a specific PLDE in $(\mathbb{F}, \sigma)$, then plug its solutions into (5) and recursively look for the remaining solutions $g = \sum_{i=0}^{b-1} g_i t^i$. Thus one can derive the solutions of a PLDE over $(\mathbb{F}(t), \sigma)$ by solving several PLDEs in $(\mathbb{F}, \sigma)$.

As already worked out in [8], this reduction leads us to a complete algorithm that solves PLDEs for $m = 1$. Moreover, using results from [2, 16, 18, 20, 8] this reduction delivers a method that eventually produces all solutions for the higher order case $m \geq 2$.

Finally, we mention a refined version of parameterized telescoping (5) ($m = 1, a_0 = -1, a_1 = 1$). If no solution exists in $\mathbb{F}$, we can decide if there exists a solution in a $\Pi\Sigma^*$-extension of $\mathbb{F}$ where the sums and products are not more deeply nested than the original expressions in the f_i. If $\mathbb{F}$ is a $\Pi\Sigma$-field, this problem has been solved in [19]. Also this algorithm carried over if $\mathbb{F}$ contains free variables; see Remark 4 for details.

Example 3. Applying our refined telescoping algorithm to the sum (4) gives the closed form

$$\begin{aligned}\sum_{k=0}^{n} kX_{n+k} = (n+1)\sum_{k=1}^{n} X_{k-1} - \sum_{k=1}^{n} kX_{k-1} \\ - (n+2)\sum_{k=1}^{n} X_{2k-2} + 2\sum_{k=1}^{n} kX_{2k-2} \\ - (n+1)\sum_{k=1}^{n} X_{2k-1} + 2\sum_{k=1}^{n} kX_{2k-1} + nX_{2n}.\end{aligned}$$

Despite being more lengthy, this representation is preferred, because it only contains indefinite single sums.

Remark 1. (Denominator bounding) In [8] we have shown that a denominator bound d can be computed if $m = 1$. For the case $m \geq 2$ this problem is not completely solved: For

Σ^*-extensions we still can compute a denominator bound, but if t is a Π-extension, we find the denominator bound only up to a power of t. The corresponding algorithms can be found in [16, Algorithm 1] by combining certain subproblems solved in [8, Corollary 1, Theorem 2, Theorem 4].

Remark 2. (Degree bounding) A degree bound can be computed if $m = 1$. For the case $m \geq 2$ we have algorithms only for various special cases [18].

Remark 3. (Degree reduction) Following the reduction recursively, one can solve PLDEs in $\mathbb{F}(t)$ if one can compute all the needed denominators (Reduction I) in $\mathbb{F}[t]$ and $\mathbb{G}(t_1)\dots(t_{i-1})[t_i]$, the degree bounds (Reduction II) in $\mathbb{F}[t]$ and $\mathbb{G}(t_1)\dots(t_{i-1})[t_i]$, and all the resulting PLDEs in $\mathbb{G}$ obtained by recursive application of Reduction III. Here the following remarks are in place.
(1) If $\mathbb{G}$ is the constant field, solving PLDEs in $\mathbb{G}$ reduces to linear algebra [20, page 805]. Also if $\mathbb{G}$ is a free difference field, PLDEs can be solved; see Section 2.2.
(2) If $m = 1$, degree and denominator bounds can be computed in $\mathbb{F}[t]$ and $\mathbb{G}(t_1)\dots(t_{i-1})[t_i]$; see Remarks 1 and 2. Hence we get a complete algorithm for solving PLDEs.
(3) If $m \geq 2$, denominator and degree bounds can be computed only partially so far. But, as worked out in [20, Theorem 5.3], the reduction leads to a method that eventually will produce all solutions of a given PLDE in $\mathbb{F}(t)$.

Remark 4. (Refined telescoping) We obtain the algorithm for this problem by combining results from [16, 18, 19, 8]. Namely, there are algorithms for computing denominator and degree bounds which have the additional property that they are extension-stable; this follows by [16, Thm. 10], [18, Thm. 17], and the fact that one can handle certain subproblems in $\mathbb{F}$; see [8, Theorems 1,3,4]. Using this fact, we obtain an algorithm that solves the refined telescoping problem; see [19, Thms. 6,8].

3. DEMOTIVATING RESULTS

With an implementation of the algorithm described in the previous section, we have searched for variations of the definite sum $\sum_{k=0}^{n} kX_{n+k}$ of Example 1. These experiments have lead us to the following theorem, which gives an explicit a priori criterion for which sequences $f_{n,k}$ a linear recurrence for the general definite sum $\sum_{k=0}^{n} f_{n,k}X_{n+k}$ is found.

THEOREM 1. *Let $(\mathbb{F}, \sigma)$ be a difference field with constant field $\mathbb{K}$, and let $f_0, \dots, f_r \in \mathbb{F}$. Then there exist $c_0, \dots, c_r \in \mathbb{K}$ and $g \in \mathbb{F}\langle x\rangle$ with*

$$\sigma(g) - g = c_0 f_0 x_0 + c_1 f_1 x_1 + \dots + c_r f_r x_r$$

if and only if there exist $b_0, \dots, b_r \in \mathbb{K}$ with

$$b_0\sigma^r(f_0) + b_1\sigma^{r-1}(f_1) + \dots + b_r f_r = 0.$$

PROOF. Suppose first that $f_0, \dots, f_r$ are such that there exist $b_0, \dots, b_r \in \mathbb{K}$ with

$$b_0\sigma^r(f_0) + b_1\sigma^{r-1}(f_1) + \dots + b_r f_r = 0. \tag{7}$$

Then $c_k := b_k$ $(k = 0, \dots, r)$ and

$$g := a_0 x_0 + a_1 x_1 + \dots + a_{r-1} x_{r-1},$$

where $a_k = -\sum_{i=0}^{k} b_i \sigma^{k-i}(f_i)$ are as required: We have

$$\begin{aligned}\sigma(g) - g &= -a_0 x_0 + \sum_{k=1}^{r-1} (\sigma(a_{k-1}) - a_k) x_k + \sigma(a_{r-1}) x_r \\ &= b_0 f_0 x_0 + \dots + b_r f_r x_r,\end{aligned}$$

because

$$\begin{aligned}-a_0 &= b_0 f_0 \\ \sigma(a_{k-1}) - a_k &= -\sum_{i=0}^{k-1} b_i \sigma^{(k-1)-i+1}(f_i) + \sum_{i=0}^{k} b_i \sigma^{k-i}(f_i) \\ &= b_k f_k \qquad (k = 1, \dots, r-1) \\ \sigma(a_{r-1}) &= -\sum_{i=0}^{r-1} b_i \sigma^{r-i}(f_i) \overset{(7)}{=} b_r f_r.\end{aligned}$$

This proves the first implication. Now, assume that there exist $c_0, \dots, c_r \in \mathbb{F}$ and $g \in \mathbb{F}\langle x\rangle$ such that

$$\sigma(g) - g = c_0 f_0 x_0 + c_1 f_1 x_1 + \dots + c_r f_r x_r. \tag{8}$$

The element g is a rational function in x_i $(i \in \mathbb{Z})$ with coefficients in $\mathbb{F}$. However, g can neither have a nontrivial denominator nor a nonlinear term, because then $\sigma(g) - g$ would have nontrivial denominator or a nonlinear term as well. Furthermore, g must be free of all x_i with $i < 0$ or $i \geq r$, for otherwise $\sigma(g) - g$ would contain some x_i with $i < 0$ or $i > r$ in mismatch with the right hand side of (8). Thus g can only have the form

$$g = a_0 x_0 + a_1 x_1 + \dots + a_{r-1} x_{r-1}$$

for certain $a_i \in \mathbb{F}$. Now

$$\sigma(g) - g = -a_0 x_0 + \sum_{k=1}^{r-1} (\sigma(a_{k-1}) - a_k) x_k + \sigma(a_{r-1}) x_r,$$

and comparing coefficients of x_k $(k = 0, \dots, r-1)$ with the right hand side of (8) gives

$$\begin{aligned}a_0 &= -c_0 f_0 \\ a_1 &= \sigma(a_0) - c_1 f_1 = -(c_0\sigma(f_0) + c_1 f_1) \\ &\vdots \\ a_{n-1} &= \sigma(a_{r-2}) - c_{r-1} f_{r-1} = -\sum_{i=0}^{r-1} c_i \sigma^{(r-1)-i}(f_i).\end{aligned}$$

Comparing finally the coefficient of x_r gives

$$c_r f_r = \sigma(a_{r-1}) = -\sum_{i=0}^{r-1} c_i \sigma^{(r-1)-i+1}(f_i),$$

and therefore we must have

$$c_0\sigma^r(f_0) + c_1\sigma^{r-1}(f_1) + \dots + c_r f_r = 0,$$

as claimed. □

For obtaining a recurrence equation of the definite sum $S_n := \sum_{k=0}^{n} f_{n,k} X_{n+k}$ via creative telescoping, we choose $f_0 = f_{n,k}$, $f_1 = f_{n+1,k}, \dots, f_r = f_{n+r,k}$ (or more precisely, corresponding difference field elements). Thus the above theorem states that a recurrence for S_n is found via creative telescoping if and only if the antidiagonal sequences $f_{i-n,n}$ $(i \in \mathbb{Z})$ are all solutions of a single homogeneous linear recurrence with constant coefficients.

Similar criteria can be obtained for sums of the form

$$S_n = \sum_{k=0}^{n} f_{n,k} X_{an+bk}$$

for any fixed $a, b \in \mathbb{Z}$. For $a = 1, b = -1$, we find the criterion that $c_0, \ldots, c_r \in \mathbb{K}$ and $g \in \mathbb{F}\langle x \rangle$ with

$$\sigma(g) - g = c_0 f_0 x_0 + c_1 f_1 x_{-1} + \cdots + c_r f_r x_{-r}$$

exist iff there exist $b_0, \ldots, b_r \in \mathbb{K}$ with

$$b_0 f_0 + b_1 \sigma(f_1) + \cdots + c_r \sigma^r(f_r) = 0,$$

If $\gcd(a, b) = 1$ (which we may assume without loss of generality by the substitution $X'_i := X_{\gcd(a,b)i}$) and $|a| > 1$, then a recurrence exists only in the trivial case $f_{n,k} \equiv 0$. The case $|a| = 1, |b| \geq 0$ leads to a restriction on the summand similar as the one stated above. The arguments for all these variations are fully analogous to the proof given above.

The theorem provides a means to obtain creative telescoping recurrences without actually executing the algorithm described in Section 2.1.

Example 4. Consider once more the definite sum $S_n = \sum_{k=0}^{n} k X_{n+k}$ of Example 1. In the notation of the theorem, we have $f_{n,k} = k$, so we immediately obtain the recurrence

$$g_{n,k+1} - g_{n,k} = k X_{n+k} - 2k X_{(n+1)+k} + k X_{(n+2)+k},$$

where

$$g_{n,k} = (k-1) X_{n+k+1} - k X_{n+k}.$$

Summing k from 0 to $n+2$ leads to the same inhomogeneous recurrence which we obtained before.

The more interesting implication of the theorem is of course that which allows us to definitely exclude the existence of creative telescoping recurrences for sums of a certain shape. For instance, the following results follow immediately.

COROLLARY 1. *For the following definite sums, no recurrence can be found via creative telescoping.*

1. $\sum_{k=0}^{n} r(k) X_{n+k}$ *for any* $r \in \mathbb{K}(x) \setminus \mathbb{K}[x]$,
2. $\sum_{k=0}^{n} \binom{n}{k} X_{n+k}$,
3. $\sum_{k=0}^{n} r(k) \prod_{i=1}^{k} X_{n+i}$ *for any* $r \in \mathbb{K}(x) \setminus \mathbb{K}[x]$. $\square$

The third sum can be brought to the form of Theorem 1 by putting $Y_k := \prod_{i=0}^{k} X_i$, for then

$$\sum_{k=0}^{n} r(k) \prod_{i=1}^{k} X_{n+i} = \sum_{k=0}^{n} r(k) Y_{n+k}/Y_n = \frac{1}{Y_n} \sum_{k=0}^{n} r(k) Y_{n+k},$$

and the factor $1/Y_n$, which is independent of k, does not affect the existence of a recurrence. The possibility of such substitutions extends the range of Theorem 1. In order to find nontrivial examples, it is necessary to focus on sums with more complicated summands.

4. MOTIVATING RESULTS

We present in this section some general identities which we have found by using the algorithm described in Section 2.1. The examples are separated into indefinite and definite sums.

4.1 Indefinite summation

Example 5. For the sum $\sum_{k=1}^{a} (-1)^k \sum_{j=1}^{k} X_j$ we find the closed form evaluation

$$\sum_{k=1}^{a} (-1)^k \sum_{j=1}^{k} X_j = \frac{1}{2} \big[(-1)^a \sum_{k=1}^{a} X_k + \sum_{k=1}^{a} (-1)^k X_k \big].$$

Specializing X_j gives the following identities.

- $X_j := \frac{1}{j}$:

$$\sum_{k=1}^{a} (-1)^k H_k = \frac{1}{2} (-1)^a H_a + \frac{1}{2} \sum_{k=1}^{a} \frac{(-1)^k}{k};$$

$H_a = \sum_{k=1}^{a} \frac{1}{k}$ denotes the harmonic numbers.

- $X_j := \binom{n}{j-1}$, $a := n+1$; see [23, Thm. 4.2]:

$$\sum_{k=0}^{n} (-1)^{k+1} \sum_{j=0}^{k} \binom{n}{j} = \frac{1}{2} (-1)^{n+1} 2^n.$$

Example 6. We find

$$\sum_{k=1}^{a} (-1)^k \binom{n}{k} \sum_{j=1}^{k} X_j = \frac{1}{n} \big[(n-a) \binom{n}{a} (-1)^a \sum_{k=1}^{a} X_k + \sum_{k=1}^{a} (-1)^k k \binom{n}{k} X_k \big].$$

In particular, in the special case $a = n$ and $X_j = \frac{1}{j^m}$ where $m \geq 1$ we get the following simplification. By [9, Prop. 2.1] we get

$$\sum_{k=1}^{n} \frac{(-1)^k}{k^{m-1}} \binom{n}{k} = -\frac{1}{(m-1)!} B_{m-1}(\ldots, (i-1)! H_N^{(i)}, \ldots)$$

where $B_m(\ldots, x_i, \ldots)$ are the complete Bell polynomials [3] and

$$H_n^{(s)} = \sum_{k=1}^{n} \frac{1}{k^s}, \quad s > 0$$

are the generalized harmonic numbers. Hence we get the closed form evaluation

$$\sum_{k=1}^{n} (-1)^k \binom{n}{k} H_k^{(m)} = -\frac{1}{n(m-1)!} B_{m-1}(\ldots, (i-1)! H_n^{(i)}, \ldots);$$

see [11, Thm. 3] The first instances are:

$$\sum_{k=1}^{a}(-1)^k\binom{n}{k}H_k = -\frac{1}{n},$$
$$\sum_{k=1}^{a}(-1)^k\binom{n}{k}H_k^{(2)} = -\frac{1}{n}H_n,$$
$$\sum_{k=1}^{a}(-1)^k\binom{n}{k}H_k^{(3)} = -\frac{1}{2n}(H_n^2+H_n^{(2)}).$$

Further indefinite summation identities are

$$\sum_{k=1}^{a}(-1)^k\Big(\sum_{j=1}^{k}X_j-\frac{X_k}{2}\Big)^2 = \frac{1}{2}(-1)^a\Big(\sum_{k=1}^{a}X_k\Big)^2-\frac{1}{4}\sum_{k=1}^{a}(-1)^kX_k^2,$$

$$\sum_{k=1}^{a}\Big(\sum_{j=1}^{k}X_j+X_k(k-1)\Big)^2 = n\Big(\sum_{k=1}^{a}X_k\Big)^2-\sum_{k=1}^{a}kX_k^2+\sum_{k=1}^{a}k^2X_k^2\Big).$$

4.2 Definite summation and summability criterions

Example 7. Similar as carried out in Examples 1 and 3 we find (and prove) with our difference field machinery the identity

$$\sum_{k=0}^{n}\Big(\sum_{i=0}^{k}X_{n-i}\Big)^2 = 2\sum_{k=0}^{n}X_k\sum_{j=0}^{k}jX_{j-1}+\sum_{k=0}^{n}X_k^2+\sum_{k=0}^{n}kX_k^2.$$

Namely, starting with $S_n=\sum_{k=0}^{n}\Big(\sum_{i=0}^{k}X_{n-i}\Big)^2$ we can compute by creative telescoping the recurrence

$$-X_{n+1}S_{n+2}+(X_{n+1}+X_{n+2})S_{n+1}-X_{n+2}S_n = -X_{n+1}X_{n+2}\big((n+2)X_{n+1}+(n+3)X_{n+2}\big).$$

Next, we solve this recurrence relation and find the solutions $1, \sum_{k=0}^{n}X_k$ for the homogeneous version and the particular solution

$$P_n=\sum_{k=0}^{n}X_k\sum_{i=0}^{k}\big(iX_{i-1}+X_i+iX_i\big);$$

since $S_n=P_n$ for $n=0,1$, it follows that $P_n=S_n$ for all n. Finally, applying our indefinite summation algorithm, we get the simplification

$$S_n=P_n=2\sum_{k=0}^{n}X_k\sum_{j=0}^{k}jX_{j-1}+\sum_{k=0}^{n}X_k^2+\sum_{k=0}^{n}kX_k^2.$$

Example 8. Consider the definite sum

$$S_n:=\sum_{k=1}^{n}\binom{n}{k}\sum_{j=1}^{k}X_j.$$

With our refined creative telescoping algorithm we can compute the recurrence

$$S_{n+1}-2S_n=X_{n+1}+\sum_{k=1}^{n}\binom{n}{k-1}X_k. \tag{9}$$

In the next step we would like to solve this recurrence. For applying our algorithms, we first have to express the definite sum

$$C_n:=\sum_{k=1}^{n}\binom{n}{k-1}X_k$$

in terms of $\Pi\Sigma^*$-expressions. To this end, we would normally compute a recurrence for that sum and afterwards solve it. However, no recurrence can be found in this case. (This can also be seen with Theorem 1, because $C_n=\sum_{k=0}^{n-1}\binom{n}{k}X_{n-k}$ after reversing the order of summation). Therefore, we have to proceed differently. Note that any solution of (9) can be decomposed into A_n+B_n where A_n and B_n fulfill the recurrences

$$A_{n+1}-2A_n=X_{n+1}, \tag{10}$$
$$B_{n+1}-2B_n=C_n. \tag{11}$$

Therefore, we can split our problem to solve (9) by solving the two recurrences in (10) and (11) separately. Then we combine the two sets of solutions to the solution set of (9). For (10) we derive the general solution

$$A_n=c_1\,2^n+2^n\sum_{k=1}^{n}\frac{X_k}{2^k}$$

where c_1 ranges over the constants. Hence, we get all solutions for (9) in the form

$$c_1 2^n+2^n\sum_{k=1}^{n}\frac{X_k}{2^k}+B_n \tag{12}$$

by taking all constants c_1 and by considering all solutions B_n of (11).
Note that (11) gives us a recipe how we can discover nice identities: Try to specialize X_k in such a way that C_n can be written in a closed form (e.g., can be represented in form of a $\Pi\Sigma^*$-extension) and that the solutions of (11) are nice. We may therefore consider (11) as a *summability criterion* for the sum S_n.

• $X_k=\frac{1}{k}$: We get easily the identity $C_n=\frac{2^{n+1}-2}{n+1}$ and find the general solution

$$B_n=c_2 2^n+2^n\big(H_n-2\sum_{i=1}^{n}\frac{1}{i2^i}\big)$$

for (11). Consequently, the general solution of (9) is

$$c_1\,2^n+2^n\sum_{k=1}^{n}\frac{1}{k2^k}+c_2 2^n+2^n\big(H_n-2\sum_{i=1}^{n}\frac{1}{i2^i}\big).$$

By choosing $c_1=c_2=0$ we obtain

$$\sum_{k=1}^{n}\binom{n}{k}H_k=2^n\big(H_n-\sum_{k=1}^{n}\frac{1}{k2^k}\big);$$

see [13, Equ. (41)].

With the same strategy we get the following identities.

- $X_k = \frac{1}{k^2}$:

$$\sum_{k=1}^{n} \binom{n}{k} H_k^{(2)} = 2^n \Big(\sum_{k=1}^{n} \frac{\sum_{j=1}^{k} \frac{2^j}{j}}{k2^k} - \sum_{k=1}^{n} \frac{H_k}{k2^k} \Big).$$

- $X_k = (k-1)!$:

$$\sum_{k=1}^{n} \binom{n}{k} \sum_{j=1}^{k} (j-1)! = 2^n \Big(\sum_{k=1}^{n} \frac{k!}{k2^k} + \sum_{k=1}^{n} \frac{k! \sum_{j=1}^{k} \frac{1}{j!}}{k2^k} - \sum_{k=1}^{n} \frac{1}{k2^k} \Big).$$

Example 9. We attack the sum

$$S_n := \sum_{k=1}^{n} \binom{n}{k}^2 \sum_{j=1}^{k} X_j$$

as in the previous example. First, we compute the recurrence

$$(n+1)S_{n+1} - 2(2n+1)S_n = (n+1)X_{n+1} + \sum_{k=1}^{n} (3n+3-2k) \binom{n}{k-1}^2 X_k.$$

This gives the general solution

$$\binom{2n}{n} \sum_{k=1}^{n} \frac{X_k}{\binom{2k}{k}} + c_1 \binom{2n}{n} + S_n^{(2)}$$

by taking all constants c_1 and all solutions of

$$(n+1)S_{n+1}^{(2)} - 2(2n+1)S_n^{(2)} = \sum_{k=1}^{n} (3n+3-2k) \binom{n}{k-1}^2 X_k.$$

Looking at this summability criterion we find the following identities.

- $X_k = \frac{1}{k}$; see [4, Equ. 2.26]:

$$\sum_{k=1}^{n} \binom{n}{k}^2 H_n = \binom{2n}{n} (2H_n - H_{2n}).$$

- $X_k = \frac{1}{k^2}$:

$$\sum_{k=1}^{n} \binom{n}{k}^2 H_n^{(2)} = \binom{2n}{n} (2H_n^{(2)} - 3 \sum_{k=1}^{n} \frac{1}{k^2 \binom{2k}{k}}).$$

Example 10. We compute for

$$S_n = \sum_{k=0}^{n} X_k \sum_{i=1}^{n-k} Y_i$$

the recurrence

$$S_{n+1} - S_n = Y_1 X_n + \sum_{k=1}^{n} Y_{n+2-k} X_{k-1}$$

and get the general solution

$$c_1 + Y_1 \sum_{k=1}^{n} X_{k-1} + S_n^{(2)}$$

by taking all solutions of

$$S_{n+1}^{(2)} - S_n^{(2)} = \sum_{k=1}^{n} Y_{n+2-k} X_{k-1}.$$

With this summability criterion we find the following identities.

- $X_k = \frac{1}{k!}, Y_k = \frac{1}{(k-2)!}$:

$$\sum_{k=0}^{n} \frac{1}{k!} \sum_{j=1}^{n-k} \frac{1}{(j-2)!} = \frac{1}{2} \sum_{k=1}^{n-1} \frac{2^k}{(k-1)!}.$$

- $X_k = H_k, Y_k = \frac{1}{k}$; see [10, Chapter 1.2.7, Exercise 22]:

$$\sum_{k=0}^{n} H_k H_{n-k} = 2n(1-H_n) + (n+1)H_n^2 - (n+1)H_n^{(2)}.$$

5. CONCLUSION

The extension of symbolic summation algorithms to free difference fields allows one the discovery of general families of summation identities, depending on unspecified sequences. We have illustrated in this paper how the $\Pi\Sigma$-theory for nested sum expressions can be extended, and we have found several general identities with the modified summation algorithms. We have also indicated (Section 3) that interesting relations can only be found for sums whose summand exceeds a certain level of sophistication; if it is too simple, then only trivial relations remain.

Though our extension itself is not very difficult, it should be remarked that it is based on a highly developed machinery for generating and solving recurrence equations with difference fields. Without using, for instance, algorithms that can optimize the nesting depth of sum expressions, we would hardly have been able to find any of the nontrivial examples in Section 4. Once general identities like those of Section 4 are available, they may be specialized in such a way that well-developed theories and/or algorithms can be applied for further processing. Example 6 points into that direction.

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