Creative Telescoping on Multiple Sums

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Abstract. We discuss the strategies and difficulties of determining a recurrence which a certain polynomial (in the form of a symbolic multiple sum) satisfies. The polynomial comes from an analysis of integral estimators derived via quasi-Monte Carlo methods.

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1 The Problem

Recently, Wiart and Wong [5] derived a formula for the covariance of an integral estimator for functions satisfying a certain decay condition, based on a quasi-Monte Carlo framework developed by Wiart, Lemieux, and Dong [4]. This formula is written as the following polynomial in x,

$$G_s(x) := \sum_{k=1}^{m+s-1} \left(\sum_{r=1}^{s} \binom{s}{r}\binom{k-1}{r-1} \frac{b-1}{(-b)^r} \sum_{i=0}^{r-1-c_m(k)} (-b)^i \binom{r-1}{i} \right) (bx)^k, \quad (1)$$

where $c_m(k) = \max(k-m, 0)$. The goal is to show that (1) is not positive for all $b, m, s \in \mathbb{N}$, $b \geq 2$ and $x \in [0, 1)$. We choose to approach this problem from the view of symbolic computation rather than analysis: we use the available symbolic tools for holonomic functions [1–3] to carry out a guess and prove strategy in order to deduce a suitable closed form for (1). This closed form contains hypergeometric series which is then used to prove the desired non-positivity statement, after applying some non-trivial manipulations and transformations. On a first glance, we note that all constituents of (1) have the property of being “holonomic” (roughly speaking, they satisfy recurrences with polynomial coefficients). The binomial coefficient, for example, can be described completely via such recurrences and some initial conditions (notably: finitely many).

This note serves the purpose of outlining the “proving” aspect, where we confirm via creative telescoping [7] that (1) satisfies a third-order linear recurrence in s (which can later be solved using [3], yielding an equivalent but simpler expression for (1)). Such a recurrence can be represented by an operator in a certain Ore algebra that maps the sequence G_s to the zero sequence: we will refer to such operators as “annihilators” of G_s. The creative telescoping algorithm, as

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implemented in the HolonomicFunctions package [2], identifies lists of operators (in the form of Ore polynomials in the above mentioned algebra) $\mathcal{P}$ and $\mathcal{Q}$ that give relations of the form

$$\sum_k P \cdot \text{summand} - \sum_k (S_k - 1) \cdot Q \cdot \text{summand} = 0, \tag{2}$$

for each $P \in \mathcal{P}$ and its corresponding $Q \in \mathcal{Q}$, where S_k denotes the forward shift operator in k. The set $\mathcal{P}$ contains the so-called "telescopers", and the set $\mathcal{Q}$ the corresponding "certificates". In a best-case scenario, all of the P's commute with the first summation (allowing us to pull it out of the sum so that we can view the elements of $\mathcal{P}$ being applied to the whole sum and not just the summand) and the second summation in (2) collapses to zero (leaving no trace of the certificate). From there, we would conclude that $\mathcal{P}$ generates a left ideal of annihilating operators for (1), that is, it generates a set of recurrences which are satisfied by (1).

However, life is not always that easy: during the application of this strategy to the particular summation problem (1), we encountered the following difficulties that are somewhat prototypical for the holonomic systems approach. This explains why, despite being automatable in principle, it still lacks a press-the-button implementation that would provide a computer proof of a claimed identity in a completely automatic way and without any human interaction.

1. The sums in (1) do not have natural boundaries in the sense that the summands do not take on non-zero values only within the given summation bounds. Thus, there is no reason to expect a priori that the inhomogeneous parts (the right sum in (2)) will simplify to zero. And indeed, we found that they did not. Thus, an additional annihilator for the right sum is required in order to homogenize the recurrence.
2. The upper boundaries contain the variable s, and the operators in $\mathcal{P}$ contain shifts in s, causing difficulties with moving $P \in \mathcal{P}$ to be outside of the sum.
3. Some of the operators in $\mathcal{Q}$ contain singularities at the boundary values so we were forced to exclude these values (which required compensation elsewhere). This is because the right sum of (2) is designed to collapse to only boundary value evaluations and we encounter problems if the summands are undefined at such values. Further issues could surface if those summands were also undefined at some intermediary value. Luckily, this was not the case here.
4. Mathematica, in its symbolic zeal, interprets the innermost sum in (1) as a hypergeometric ${}_2F_1$ series and the second innermost sum as a DifferenceRoot. While the values of the ${}_2F_1$ function match with our sum within the domain in question, there are still an infinite number of values for which it doesn't. The difference root is Mathematica's version of a recurrence together with initial values, but unfortunately not helpful for our purposes because it is incompatible with HolonomicFunctions and does not support multivariate recurrences that are needed for creative telescoping.

2 A Computer Proof

This section illustrates how to overcome the difficulties listed in the previous section and how to use the computer to prove our main result. We envision that this discussion leads to a deeper understanding of the practical issues of applying the holonomic systems approach, and that it will be useful for different applications in the future. The Mathematica notebook illustrating our computations can be found in the online supplementary material [6] for the paper [5].

Theorem 1. *For $b, m, s \in \mathbb{N}, b \geq 2$, the polynomial* (1) *satisfies the recurrence*

$$\begin{aligned}
&(s+2)(bx-1)\cdot G_{s+3}\\
&+(m(bx-1)(x-1)+bsx(x-2)+bx(x-3)-s(2x-3)-3x+5)\cdot G_{s+2}\\
&-(x-1)(bmx+bsx+bx+mx-2m+sx-3s+x-4)\cdot G_{s+1}\\
&+(x-1)^2(m+s+1)\cdot G_s=0.
\end{aligned}$$

Proof strategy. The steps that we invoke are as follows (here we only summarize the main ideas and omit all of the technicalities). We also perform the service of illustrating how computers and humans interact, by highlighting (in brackets) when paper-and-pencil reasoning is used and when automation is applied.

1. We employ the Guess package [1] (computer) to predict the recurrence which (1) satisfies, by using sufficiently generic evaluations of (1). This step could be postponed to the end, but here it gives us confidence that a sufficiently nice recurrence exists, and serves as an additional sanity check.
2. The summation (1) is separated into two parts (human) in order to remove the max function in the upper limit of the innermost sum.

   After a mild simplification, these two parts look as follows:

$$G_s^{(1)} := -\sum_{k=1}^{m+s-1}\sum_{r=1}^{s}\binom{s}{r}\binom{k-1}{r-1}\left(\frac{b-1}{b}\right)^r (bx)^k,$$
$$G_s^{(2)} := \sum_{k=m+1}^{m+s-1}\sum_{r=1}^{s}\binom{s}{r}\binom{k-1}{r-1}\frac{1-b}{(-b)^r}\sum_{i=r-(k-m)}^{r-1}(-b)^i\binom{r-1}{i}(bx)^k.$$

   We write this out to highlight that they don't have natural boundaries. In particular, if $k > m+s-1$, then there is no reason to expect that either of the inner sums would be zero, which may cause the inhomogeneous parts in (2) to survive.
3. The sums $G_s^{(1)}$ and $G_s^{(2)}$ are treated separately, applying the method of creative telescoping and closure properties first to the inner sum of each to obtain its annihilator and then to the outer sum (computer). We briefly illustrate how to tackle the issues mentioned in the first section:

⋆ We found that some certificates Q (computer) contain singularities on the boundary values of the inner sum. This implies that the limits of the sum must be adjusted so that we avoid evaluating at those points. To illustrate this more simply, suppose $Q = \frac{1}{r-s-1} \cdot S_s$ and $F(s,k,r)$ is our summand. Then it is clear that the telescoping sum

$$\sum_{r=1}^{s} (S_r - 1) \cdot Q \cdot F(s,k,r) = (Q \cdot F)(s,k,s+1) - (Q \cdot F)(s,k,1)$$

cannot be determined. We instead adjust the upper summation bound to $r = s-1$ and accordingly compensate (human) with additional terms that are added to the inhomogeneous parts obtained from telescoping.

⋆ We also found that the telescoper P (computer) does not commute with our summation. To simplify this illustration, suppose $P = S_s^2$, the second-order shift operator in s, and write the summand as $H(s,k)$. Then

$$P \cdot \sum_{k=1}^{m+s-1} H(s,k) = \sum_{k=1}^{m+s+1} H(s+2,k) \neq \sum_{k=1}^{m+s-1} H(s+2,k) = \sum_{k=1}^{m+s-1} P \cdot H(s,k).$$

This implies a necessary compensation of terms (human), namely, $-H(s+2, m+s)$ and $-H(s+2, m+s+1)$, to be added to the inhomogeneous part, as well as any other terms resulting from the singularity analysis above.

⋆ Lastly, to deal with Mathematica's enthusiasm for replacing our sums with their version of closed forms (computer) which match the values on our domain (but not necessarily anywhere else), we take advantage of the fact that we can write all of the inhomogeneous parts as different shifts and substitutions of the given summand. More precisely, the total of these parts can be expressed as an operator applied to the summand, followed by a substitution. Then, an annihilator for the inhomogeneous parts can be derived (human) by applying the closure properties "application of an operator" and "integer-linear substitution". In this way, we completely avoid dealing with expressions like ${}_2F_1$'s and DifferenceRoots.

The above treatments enable us to compute annihilators for $G_s^{(1)}$ and $G_s^{(2)}$, by multiplying (on the left) the annihilator of all of the inhomogeneous parts to the telescoper P that was pulled out of the left summand of (2).

4. We use closure properties to determine the annihilating ideal for (1): the sum of holonomic functions is still holonomic, so the annihilator of $G_s^{(1)} + G_s^{(2)}$ can be deduced by executing (computer) the corresponding algorithm.
5. Comparing our result, a fifth-order recurrence with considerably large coefficients, with the guessed third-order recurrence reveals that creative telescoping and closure properties overshot. Nevertheless, by showing that the fifth-order operator is a left multiple of the third-order one (computer), and by comparing initial values (human), we can conclude the assertion of Theorem 1 is true.

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