Positivity of the Gillis-Reznick-Zeilberger rational function

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Abstract

In this note we provide further evidence for a conjecture of Gillis, Reznick, and Zeilberger on the positivity of the diagonal coefficients of a multivariate rational function. Kauers had proven this conjecture for up to 6 variables using computer algebra. We present a variation of his approach that allows us to prove positivity of the coefficients up to 17 variables using symbolic computation.

Keywords: Positivity, cylindrical decomposition, rational function, symbolic summation

1 Introduction

The problem of deciding whether a given multivariate rational function has all positive coefficients in its Taylor expansion around the origin has attracted mathematicians of different fields over the past (at least) 80 years. One of the early results is due to Szegő [17] showing that $\big((1-x)(1-y)+(1-x)(1-z)+(1-y)(1-z)\big)^{-\beta}$ has all positive coefficients for $\beta > \frac{1}{2}$. A four-variable long-standing open conjecture was known as the Lewy-Askey problem and concerned the non-negativity of

$$\big(1-x-y-x-w+\tfrac{2}{3}(xy+xz+xw+yz+yw+zw)\big)^{-1}.$$

This conjecture was settled only in 2014 by Scott and Sokal [14]. More references can be found, e.g., in Straub and Zudilin's recent paper on positivity of rational functions and their diagonals [15]. The family of functions considered in this paper is also discussed therein.

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Askey and Gasper [2] showed in 1977 that $(1-(x+y+z)+4xyz)^{-\beta}$ has positive power series coefficients for $\beta \geq (\sqrt{17}-3)/2$. In 1983, Gillis, Reznick, and Zeilberger [5] gave a short proof of this result using "elementary methods" . In this very paper, they conjectured that $(1-(x_1+x_2+\cdots+x_r)+r!x_1\cdots x_r)^{-1}$ has positive power series coefficients for $r \geq 4$. They also claimed that positivity of the diagonal coefficients implies positivity throughout, but "the proof is rather long and we omit it here". For the diagonal coefficients they provided a neat formula in terms of a binomial sum.

In 2007, Kauers [7] showed positivity on the diagonal for $r = 4, 5, 6$ using symbolic computation and the binomial sum. His approach follows a method introduced by Gerhold and himself [4] for automatically proving inequalities for expressions satisfying very general recurrences in a discrete parameter. He states that he believes "that for any specific value of r it is possible to obtain a similar proof, but the runtime requirements for the computations grow drastically and with currently available machines we were not able to go beyond $r = 6$ with reasonable effort".

In this paper, we present a way to circumvent the main computational bottleneck in Kauers' computations and are able to prove positivity for values up to $r = 17$. We believe that this approach could be followed to provide evidence for the full conjecture up to higher number of variables. Independent of this problem, we propose that this or a similar method could be applied to other open problems in positivity leading to an automatic proof.

Concerning notation, we follow Kauers [7] (note that the roles of r and n are reversed compared to Gillis, Reznick, and Zeilberger). We start by introducing the full problem and collecting some simple observations about the full rational function, before we turn to the proof for the diagonal in section 4.

2 The Gillis-Reznick-Zeilberger rational function

The r-variate rational function introduced by Gillis, Reznick, and Zeilberger [5] is

$$A_r(x_1, x_2, \ldots, x_r) = \frac{1}{1-(x_1+x_2+\cdots+x_r)+r!x_1x_2\ldots x_r}. \tag{1}$$

Note that this function, that we refer to as GRZ-function in the following, is symmetric. We denote the coefficients in its Taylor series expansion by

a_r, i.e.,

$$A_r(x_1, x_2, \ldots, x_r) = \sum_{n_1,\ldots,n_r \geq 0} a_r(n_1, \ldots, n_r)\, x_1^{n_1} \cdots x_r^{n_r}. \tag{2}$$

The motivation to consider this particular family of rational functions goes back to the Askey-Gasper rational function. A particular case of this result is that

$$1/(1 - (x + y + z) + 4xyz)$$

has only positive power series coefficients. Gillis, Reznick, and Zeilberger were interested in deciding for which α the multivariate rational function

$$1/(1 - (x_1 + \cdots + x_r) + \alpha x_1 \cdots x_r)$$

is non-negative in this sense. They observed that, since the coefficient of $x_1 \cdots x_r$ is $a_r(1, \ldots, 1) = r! - \alpha$, clearly one must have $\alpha \leq r!$ and conjectured that for $r \geq 4$, $\alpha = r!$. The restriction on r is necessary: we have that $A_1(x_1) = 1$, but then

$$A_2(x_1, x_2) = 1 + x_1 + x_2 + x_1^2 + x_2^2 - x_1 x_2^2 - x_1^2 x_2 + \ldots,$$

and for $A_3(x_1, x_2, x_3)$ the first negative coefficient is $a_3(2, 2, 1) = a_3(2, 1, 2) = a_3(1, 2, 2) = -6$. In particular, we also have that $a_2(2, 2) = -2$ and $a_3(2, 2, 2) = -18$.

A recurrence relation for the multivariate sequence $a_r(n_1, n_2, \ldots, n_r)$ can be obtained by equating (1) and (2), multiplying by the denominator of the rational function, and comparing coefficients yielding,

$$\begin{aligned} a_r(n_1 + 1, n_2 + 1, \ldots, n_r + 1) = {} & a_r(n_1, n_2 + 1, \ldots, n_r + 1) + \ldots \\ & \cdots + a_r(n_1 + 1, n_2 + 1, \ldots, n_{r-1} + 1, n_r) \\ & \cdots - r! a_r(n_1, \ldots, n_r), \end{aligned}$$

with constant coefficient $a_r(0, \ldots, 0) = 1$. Let $e_{m_1,\ldots,m_k}$ be the vector of length r with values 1 at positions m_j and 0 otherwise. From the recurrence (or equivalently from coefficient comparison) it is easy to see that $a(e_{m_1,\ldots,m_k}) = k!$ for $1 \leq k \leq r - 1$, and that $a_r(1, \ldots, 1) = 0$. Furthermore, any of its coefficients that is zero in at least one component can be computed by the recurrence

$$a_r(n_1, n_2, \ldots, n_r) = a_r(n_1 - 1, n_2, \ldots, n_r) + \cdots + a_r(n_1, n_2, \ldots, n_{r-1}, n_r - 1),$$

with $a_r(\dots,-1,\dots)=0$. This can be seen most easily from the coefficient comparison after clearing denominators. Hence, $a_r(m_1,\dots,0,\dots,m_r)\geq 0$ for $m_j\geq 0$.

Gillis, Reznick, and Zeilberger state in Proposition 3 that non-negativity of the diagonal is a sufficient condition for non-negativity of the full GRZ-function. Note that, rewriting the recurrence relation in the form

$$a_r(n_1+1,n_2+1,\dots,n_r+1)+r!a_r(n_1,\dots,n_r)=\\ a_r(n_1,n_2+1,\dots,n_r+1)+\cdots+a_r(n_1+1,n_2+1,\dots,n_{r-1}+1,n_r),$$

and using symmetry again, we may quickly conclude that

$$a_r(m,\dots,m)\geq 0 \quad\Longrightarrow\quad a_r(m,m+1,\dots,m+1)\geq 0$$

for $m\geq 0$. This is a simple result of positivity on the diagonal extending to off-diagonal positivity. Besides stating this, we make no attempt on proving Proposition 3 of [5]. Below, we start from the closed form provided by Gillis, Reznick, and Zeilberger

$$a_r(n):=a_r(n,\dots,n)=\sum_{k=0}^{n}(-1)^k\frac{(rn-(r-1)k)!(r!)^k}{(n-k)!^r k!}, \tag{3}$$

and show how to prove non-negativity of this binomial sum for r up to 17 using computer algebra.

3 The Gerhold-Kauers method and previous results

Gerhold and Kauers [4] introduced in 2005 a method to prove positivity of expressions involving a discrete parameter along which they satisfy some type of difference equation. The proof proceeds by induction along this discrete parameter and uses Cylindrical Algebraic Decomposition (CAD) on a generalized induction formula. CAD is a method that was introduced to solve the problem of quantifier elimination over the theory of real numbers [3]. Given a logical formula on polynomial expressions involving quantifiers, CAD computes a logically equivalent, quantifier-free formula. In the case when there are no free variables, this formula is just one of the logical constants true or false. Else, it gives a normalized representation of the given expression in terms of the free variables.

The Gerhold-Kauers method has been applied successfully to several problems, see, e.g., [1, 10, 8]. There are cases where the original approach fails to succeed, but with a little variation of the theme, CAD can still be applied to prove non-trivial, non-polynomial inequalities [6]. In 2007 Kauers presented a modification [7] that he applied to prove positivity of $a_r(n)$ for $r = 4, 5, 6$ and $n \geq 0$. We present a variant of this approach that allows us to proceed up to $r = 17$.

Let $a_r(n)$ be the binomial sum defined by (3). Then, it is well known that for any fixed integer r this sum satisfies a linear recurrence with polynomial coefficients of some order say d,

$$c_0(n)a_r(n) + c_1(n)a_r(n+1) + \cdots + c_d(n)a_r(n+d) = 0. \tag{4}$$

Such a recurrence can be derived automatically using Zeilberger's algorithm [19, 18, 20]. In our computations below, we use the Paule-Schorn [9] implementation in Mathematica, but there exist other packages such as, e.g., gfun [13] in Maple.

The original method by Gerhold and Kauers proceeds by inductive proof. In our case, we would seek to prove that for all $n \geq 0$,

$$a_r(n) \geq 0 \wedge a_r(n+1) \geq 0 \wedge \cdots \wedge a_r(n+d-1) \geq 0 \Rightarrow a_r(n+d) \geq 0.$$

The recurrence (4) can be used to relate $a_r(n+d)$ to lower shifts with polynomial coefficients. Still, the task at hand is not yet a polynomial expression that can be handed over to CAD. For this we build the generalized induction step formula,

$$\begin{aligned} &\forall y_0, y_1, \ldots, y_{r-1}, x \colon x \geq 0 \wedge y_0 \geq 0 \wedge y_1 \geq 0 \wedge \cdots \wedge y_{r-1} \geq 0 \\ &\qquad\qquad \wedge c_0(x)y_0 + \ldots c_{r-1}(x)y_{r-1} + c_r(x)y_r = 0 \Rightarrow y_r \geq 0. \end{aligned}$$

This formula is certainly more general than what we need for the induction to be proven. It has the advantage, however, that CAD can decide whether it is true or not. If it is true, then this yields the induction step in the particular case for $a_r(n)$. If the generalized statement is false, this yields no information on the sequence or whether an inductive proof is possible or not. In that case, the induction hypothesis is extended by one and the new generalized induction formula is checked using CAD. In every such step, another initial value is being checked. If a counterexample is found, the inequality is disproven. Else, this process may be continued indefinitely - thus it is rather a method and not an algorithm in the strict sense.

Kauers observed that this approach did not seem to work for showing positivity of the GRZ-function. Hence he modified it [7]. Instead of proving positivity of the given sequence, he turned to proving the stronger property of increasing monotonically using the original method. Additionally he introduced a degree of freedom, by considering the sequence $\beta^{-n}a_r(n)$ for some positive parameter β. Clearly, if sufficiently many initial values are positive and $\beta^{-n}a_r(n)$ is an increasing sequence, positivity of $a_r(n)$ follows. For this new task a generalized induction step formula is built and following the notation above, this formula looks like

$$\begin{aligned}\forall y_0,\ldots,y_d\,\forall x \geq 0\colon\ (&y_0 > 0 \wedge y_1 > \beta y_0 \wedge \cdots \wedge y_{d-1} > \beta y_{d-2} \\ &\wedge c_0(x)y_0 + c_1(x)y_1 + \cdots + c_d(x)y_d = 0) \Rightarrow y_d > \beta y_{d-1}.\end{aligned} \tag{5}$$

A CAD computation [16] can determine whether β exists such that the formula above holds and at the same time compute a range of feasible values.

Kauers [7] results show that for $r = 4, 5, 6$ such a proof is possible for $\beta > \beta_0$ with $\beta_0 \simeq 42.04, 138.9$, and 715.5, respectively. As mentioned in the introduction, he states that he believes that this approach will work for any particular value of r, but current computers (back in 2007) do not allow to go beyond $r = 6$ in a reasonable way.

Typically for the Gerhold-Kauers method (or variants), the computational bottleneck is the CAD computation. It is doubly exponential in the number of variables, depends badly on the polynomial degrees, and shows this behaviour not only in theory, but often in practice. Our computations indicate that the most expensive part in the calculations is determining the range for β. Once the parameter assumes a particular value, the CAD computations are relatively fast. Hence we separate finding β_0 from using it and choose a cheaper way to determine a sufficient bound for β.

4 Positivity on the diagonal

Recall that the binomial sum (3) we consider is given by

$$a_r(n) = \sum_{k=0}^{n}(-1)^k \frac{(rn-(r-1)k)!(r!)^k}{(n-k)!^r k!}.$$

For fixed r, the sequence $(a_r(n))_{n\geq 0}$ satisfies a linear recurrence with polynomial coefficients, which can be computed automatically (for any specific choice of r) using algorithms for symbolic summation. We used creative telescoping following Zeilberger's algorithm and computed these recurrences up to $r = 17$. From these values we observed that for each r, $a_r(n)$ satisfies a fully balanced recurrence of order r with all coefficients of equal degree $d(r) = \binom{r}{2}$, say

$$c_0(n)a_r(n)+c_1(n)a_r(n+1)+\cdots+c_r(n)a_r(n+r) = 0, \quad \deg c_i(n) = \binom{r}{2}. \tag{6}$$

Let us define the characteristic polynomial of this recurrence as

$$\chi_r(x) = \mathrm{lc}_y\left(c_0(y) + c_1(y)x + \cdots + c_r(y)x^r\right).$$

Then, our experiments showed that β_0 can be chosen as the smallest positive root of the characteristic polynomial. For smaller values of r (i.e., $r = 4, 5, 6$), we find that actually β has to be chosen in some closed interval $\beta_0 \le \beta \le \beta_1$. For instance for $r = 4$ we find that β_0 is the smallest positive root of the characteristic polynomial

$$\chi_4(x) = -32x^4 + 5120x^3 - 110592x^2 - 1769472x - 10616832, \quad \beta_0 \simeq 42.04,$$

and β_1 is the largest positive root of $11x^4 - 1209x^3 + 13581x^2 + 100440x + 171072$ with approximate value $\beta_1 \simeq 96.0473$. This value is smaller than the largest positive root of $\chi_r(x)$ which is approximately 129.99. The upper bound is not a root of the characteristic polynomial, but the range $[\beta_0, \beta_1]$ appears to be big enough to pick a suitable value for β even without its knowledge. As a simple choice we go with $\beta = \lceil \beta_0 \rceil$ which works well in all cases. It might still be that choosing larger values decreases the computation time of CAD a bit. Summarizing, our procedure is as follows:

1. Compute a recurrence relation for $a_r(n)$;
2. Compute the characteristic polynomial $\chi_r(x)$;
3. Choose β_r as the ceiling of the smallest positive root of $\chi_r(x)$;
4. Prove that $\beta_r^{-n} a_r(n)$ is monotonically increasing using Gerhold-Kauers.

Following this approach we are able to prove positivity of the diagnoal coefficients up to (at least) $r = 17$.

Theorem 1. *Let $a_r(n) = \sum_{k=0}^{n} (-1)^k \frac{(rn-(r-1)k)!(r!)^k}{(n-k)!^r k!}$. Then $a_r(n) > 0$ for $r = 4, \ldots, 17$ and $n \ge 2$.*

Proof. Apply the procedure described above and use your favourite implementation of CAD to prove the generalized induction step formula (5) with the following values for β,

r	β_r
4	43
5	139
6	716
7	4586
8	34565
9	297860
10	2880692

r	β_r
11	30853466
12	362227628
13	4623407173
14	63724202836
15	943044296791
16	14911669278343
17	250870733898940

To finish the proof, it remains to check the initial values, i.e., to verify that $a_r(n+1) > \beta_r a_r(n)$ for $n = 2, \ldots, r+1$ and $r = 4, \ldots, 17$. The recurrences for $r = 4, \ldots, 17$ are available for download at

http://www.risc.jku.at/people/vpillwei/grz/

□

Note that in section 2 we showed that $a_r(0) = 1$ and $a_r(1) = 0$. Together with this, Theorem 1 gives non-negativity of $a_r(n)$ for all $n \geq 0$ and $r = 4, \ldots, 17$.

As r grows, the computation times spent for CAD certainly increases, but so does also the memory and time consumption for obtaining the recurrence relations. Up to $r = 9$, we used the Paule and Schorn-implementation [9] of Zeilberger's algorithm to determine the recurrences. The computational effort for this step grows rapidly, hence after that we employed a Guess-and-Prove strategy that we outline briefly. Let us denote by

$$s_r(n,k) = (-1)^k \frac{(rn-(r-1)k)!(r!)^k}{(n-k)!^r k!},$$

the summand in (3) and recall that Zeilberger's algorithm proceeds by determining a creative telescoping relation of the form,

$$\begin{aligned} c_0(n)s_r(n,k) + c_1(n)s_r(n+1,k) + \ldots \\ \cdots + c_r(n)s_r(n+r,k) = \Delta_k\left(R_r(n,k)s_r(n,k)\right), \end{aligned} \tag{7}$$

with polynomial coefficients $c_j(n)$ depending only on n and not on the summation variable k, a rational function $R_r(n,k)$ referred to as certificate, and Δ_k denoting the forward difference operator in k, i.e., $\Delta_k(b(k)) = b(k+1) - b(k)$. Under suitable assumptions, upon summing over (7), the right hand side telescopes to zero and we are left with a linear recurrence satisfied by $a_r(n)$ with the polynomial coefficients $c_j(n)$. Zeilberger's algorithm need not find the minimal recurrence for a given sequence. Still, the calculations we performed for $r = 4, \ldots, 9$ provided some insight on the telescoping recurrences, such as its order and the degree of its coefficients. We use this knowledge in guessing to compute a recurrence of order r with degree $\binom{r}{2}$. In order to verify the guessed recurrence, we only need to compute the certificate $R_r(n,k)$. To do this, we divide the telescoping equation by $s_r(n,k)$ and obtain

$$\begin{aligned} c_0(n) + c_1(n)\frac{s_r(n+1,k)}{s_r(n,k)} + \cdots + c_{r-1}(n)\frac{s_r(n+r-1,k)}{s_r(n,k)} \\ + c_r(n)\frac{s_r(n+r,k)}{s_r(n,k)} = R_r(n,k+1)\frac{s_r(n,k+1)}{s_r(n,k)} - R_r(n,k). \end{aligned}$$

The forward shift quotients $s_r(n+j,k)/s_r(n,k)$ and $s_r(n,k+1)/s_r(n,k)$ can be computed explicitely and so can their common denominator. The cases $r = 4, \ldots, 9$ indicate that the certificate is of the form

$$R_r(n,k) = (-1)^r \; P_r(n,k) \Bigg/ \prod_{i=1}^{r} (n-k+i)^r \;,$$

for some bivariate polynomial $P_r(n,k)$ that is of the form

$$P_r(n,k) = \sum_{j=0}^{d} \sum_{i=1}^{d_1} \gamma(i,j) k^i n^j + \sum_{j=d+1}^{d_2} \sum_{i=1}^{d_2-j+1} \gamma(i,j) k^i n^j,$$

with degrees

$$d = d(r) = \binom{r}{2}, \quad d_1 = d_1(r) = r^2, \quad d_2 = d_2(r) = \tfrac{1}{2}(3r+1)(r-1).$$

Note that $d = d_2 - d_1 + 1$ and that the number of variables $\gamma(i,j)$ is $r^2(2r^2 - r + 1)/2$. With this ansatz, the certificate can be computed from the guessed recurrence explicitely (if it exists), thus proving the recurrence.

Gillis, Reznick, and Zeilberger supported their conjecture by computing $a_r(n)$ for $r = 4$ and $1 \leq n \leq 220$. In this range they noticed that $a_4(n)$ is increasing "monotonically and appears to have exponential growth". From our observations this seems to hold also for larger values of r with $a_r(n) \sim \alpha_r^n n^{(r-1)/2}$ as $n \to \infty$, with α_r the largest positive root of $\chi_r(x)$. Also the coefficients in the recurrence and the certificate are growing with r, e.g., for $r = 11$ there are 14036 coefficients $\gamma(i,j)$ with absolute values ranging in size in the order of 10^{121} to 10^{272}. This results in a characteristic polynomial with integer coefficients of the form

$$\begin{aligned} \chi_{11}(x) = x^{11} &- 2.8487 \times 10^{11} x^{10} + 8.7634 \times 10^{16} x^9 + 1.0494 \times 10^{25} x^8 \\ &+ 8.3779 \times 10^{32} x^7 + 4.6819 \times 10^{40} x^6 + 1.8689 \times 10^{48} x^5 \\ &+ 5.3285 \times 10^{55} x^4 + 1.0635 \times 10^{63} x^3 + 1.4150 \times 10^{70} x^2 \\ &+ 1.1297 \times 10^{77} x + 4.0993 \times 10^{83} \end{aligned}$$

with the smallest positive root bounded above by $\beta_{11} = 30853466$. For the largest positive root in this case we have that $\lfloor \alpha_{11} \rfloor = 284872278055$. Note that, for inductively showing monotonicity, it is necessary to consider the sequence $a_r(n)/\beta_r^n$, i.e., to scale the sequence down. Intiuitively one might expect that the role of the parameter β is to accentuate the monotonicity, not to dampen it, or that the sequence needs to be normalized to largest eigenvalue $\alpha_r = 1$. At least for this example, neither is the case.

5 Concluding remarks

We have presented a proof for the positivity of the Gillis-Reznick-Zeilberger rational function (or at least its diagonal) for $r = 4, \ldots, 17$, thus providing more evidence for the full conjecture. Besides that, a goal of this work was to point out a practical improvement of Kauers' approach by separating the finding of the parameter β from using it in the proof. For this, the initial approach was to consider the limiting C-finite recurrence

$$\mathrm{lc}_y \left(c_0(y)\tilde{a}_r(n) + c_1(y)\tilde{a}_r(n+1) + \cdots + c_r r(y)\tilde{a}_r(n+r) \right) = 0,$$

where lc_y denotes the leading coefficient w.r.t. y. Then we used Kauers' method applied to the sequence $\tilde{a}_r(n)$ to determine a candidate for β_r. Doing this, we found that in the case of the GRZ-rational function the smallest positive root of the characteristic polynomial is such a candidate.

We believe that considering the limiting C-finite sequences to determine parameters is a viable approach at least for balanced recurrences, i.e., recurrences where the leading and trailing coefficient have the same polynomial degree d and all other coefficients degrees at most d. Besides determining parameters, these sequences could also be used to decide which strategy is optimal: the original Gerhold-Kauers approach with increasing the induction hypothesis if necessary; introducing a parameter and proving monotonicity; considering shifted subsequences (for details see [11, 12]); or combinations of these approaches. Many problems are in theory accessible to computer algebra, but fail solely because of the computational complexity being presently too high. We see these approaches as ways to circumvent this restriction and prove these problems using symbolic computation.

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