Experiments with a Positivity-Preserving Operator

Manuel Kauers and Doron Zeilberger

CONTENTS

We consider some multivariate rational functions that have (or are conjectured to have) only positive coefficients in their series expansion. We consider an operator that preserves positivity of series coefficients, and apply the inverse of this operator to the rational functions. We obtain new rational functions that seem to have only positive coefficients, whose positivity would imply positivity of the original series, and that, in a certain sense, cannot be improved any further.

1. INTRODUCTION

Are all the coefficients in the multivariate series expansion about the origin of

$$\frac{1}{1-x-y-z-w+\frac{2}{3}(xy+xz+xw+yz+yw+zw)}$$

positive? Nobody knows. For a similar rational function in three variables, Szegő [Szegő 33] has shown positivity of the series coefficients using involved arguments. His dissatisfaction with the discrepancy between the simplicity of the statement and the sophistication of the methods he used in his proof has motivated further research about positivity of the series coefficients of multivariate rational functions. For several rational functions, including Szegő's, there are now available simple proofs of the positivity of their coefficients. For others, including the one quoted above [Askey and Gasper 72], the positivity of their coefficients are long-standing and still open conjectures.

In this paper, we consider the positivity problem in connection with the operator T_p ($p \geq 0$) defined as follows:

$$T_p\colon \mathbb{R}[\![x_1,\dots,x_n]\!] \to \mathbb{R}[\![x_1,\dots,x_n]\!],$$
$$(T_p f)(x_1,\dots,x_n) := \frac{f\left(\frac{px_1}{1-(1-p)x_1},\dots,\frac{px_n}{1-(1-p)x_n}\right)}{(1-(1-p)x_1)\cdots(1-(1-p)x_n)}.$$

By construction, the operator T_p preserves positive coefficients for every $0 \leq p \leq 1$; that is, if a power series

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f has positive coefficients, then the power series $T_p f$ has positive coefficients as well, for every $0 \le p \le 1$. For example, via

$$T_{1/2}\left(\frac{1}{1-x-y-z+4xyz}\right) = \frac{1}{1-x-y-z+\frac{3}{4}(xy+xz+yz)},$$

positivity of the former rational function [Askey and Gasper 77] implies positivity of Szegő's rational function [Szegő 33]. This is a fortunate relation, because the positivity of the former can be shown directly by a simple argument [Gillis and Kleeman 79], while this is not so easy for the latter [Kauers 07]. (A different positivity-preserving operator also connecting these two functions is given in [Straub 08].)

This suggests applying the operator T_p "backward" to a rational function f for which positivity of the coefficients is conjectured, in the hope that this leads to a rational function that again has positive coefficients and for which positivity of the coefficients is easier to prove.

We present some empirical results in this direction. Our results may or may not lead to rigorous proofs of some open problems. In either case, we also find them interesting in their own right.

2. SHARP IMPROVEMENTS

Given a rational function f, we are interested in parameters $p \in [0, 1]$ such that $T_p^{-1} f$ has positive series coefficients. Because of $T_p^{-1} = T_{1/p}$, this is equivalent to asking for parameters $p \ge 1$ such that $T_p f$ has positive series coefficients. Clearly, the set of all $p \ge 0$ such that $T_p f$ has positive coefficients forms an interval $[0, p_{\max})$ with a characteristic upper bound $p_{\max}$ for each particular f. Computer experiments have led to the following empirical results.

Empirical Result 2.1. *Let $f(x, y, z) = 1/(1 - x - y - z + 4xyz)$. Let p_0 be the real root of $2x^3 - 3x^2 - 1$ with $p_0 \approx 1.68$. Then $p_0 = p_{\max}$.*

Evidence:

1. The bound $p_{\max}$ cannot be larger than p_0, because the particular coefficient $\langle xyz\rangle T_p f = 1 + 3p^2 - 2p^3$ fails to be positive for $p \ge p_0$.

2. CAD (cylindrical algebraic decomposition) computations confirm that all terms $\langle x^n y^m z^k\rangle T_p f$ with $0 \le n, m, k \le 50$ are positive for any $0 < p < p_0$.

3. For $p = 2430275/1448618$, all terms $\langle x^n y^m z^k\rangle T_p f$ with $0 \le n, m, k \le 100$ are positive. This p is the fifteenth convergent to p_0 and only about 10^{-14} smaller than this value.

4. For each specific choice of m, k, the terms $\langle x^n y^m z^k\rangle T_p f$ are polynomials in n (and p) of degree $m + k$ with respect to n. For $0 \le m, k \le 10$, CAD computations confirm that these are positive for all $n \ge 1$ and all $0 < p < p_0$.

□

Empirical Result 2.2. *Let $f(x, y, z, w) = 1/(1 - x - y - z - w + \frac{2}{3}(xy + xz + xw + yz + yw + zw))$. Let p_0 be the real root of $x^4 - 6x^2 - 3$ with $p_0 \approx 2.54$. Then $p_0 = p_{\max}$.*

Evidence:

1. The bound $p_{\max}$ cannot be larger than p_0, because the particular coefficient $\langle xyzw\rangle T_p f = 3 + 6p^2 - p^4$ fails to be positive for $p \ge p_0$.

2. CAD computations confirm that all terms $\langle x^n y^m z^k w^l\rangle T_p f$ with $0 \le n, m, k, l \le 25$ are positive for any $0 < p < p_0$.

3. For $p = 730647/287378$, all terms $\langle x^n y^m z^k w^l\rangle T_p f$ with $0 \le n, m, k, l \le 240$ are positive. This p is the fifteenth convergent to p_0 and only about 10^{-12} smaller than this value.

4. For each specific choice of m, k, l, the terms $\langle x^n y^m z^k w^l\rangle T_p f$ are polynomials in n (and p) of degree $m+k+l$ with respect to n. For $0 \le m, k, l \le 5$, CAD computations confirm that these polynomials are positive for all $n \ge 1$ and all $0 < p < p_0$.

□

For the rational function f considered in Empirical Result 2.2, our hope that a direct proof for the positivity of $T_{p_{\max}} f$ could be found more easily than for f itself was in vain. However, some "suboptimal" values of p do lead to rational functions that have a promising shape. For instance, we found that

$$T_{\sqrt{3}}\Big(\frac{1}{1-x-y-z-w+\frac{2}{3}(xy+xz+xw+yz+yw+zw)}\Big) = \frac{1}{1-x-y-z-w+2(xyz+xyw+xzw+yzw)+4xyzw}.$$

Also note that it seems to be a coincidence that $p_{\max}$ is determined by the coefficient of $xyzw$ in $T_p f$, because this does not hold in the expansion of

$$f(x, y, z, w) = \frac{1}{1-x-y-z-w+\frac{64}{27}(xyz+xyw+xzw+yzw)},$$

which is conjectured to have positive coefficients [Kauers 07]. Here we have $p_{\max} < 1.66$, by inspection of the coefficients $\langle x^n y^m z^k w^l\rangle T_p f$ for $0 \le n, m, k, l \le 100$, while $\langle xyzw\rangle T_p f = -\frac{13}{27}p^4 - \frac{40}{27}p^3 + 6p^2 + 1$ is positive for $p < 2.36$.

3. ASYMPTOTICALLY POSITIVE COEFFICIENTS

Inspection of initial coefficients of

$$\frac{1}{1 - x - y - z - w + \frac{64}{27}(xyz + xyw + xzw + yzw)}$$

suggests values for $p_{\max}$ that become smaller and smaller as the number of initial values taken into consideration increases. Is the "real" value $p_{\max}$ determined by the asymptotic behavior of the coefficients for general p?

Clearly, it is hard to extract conjectures about asymptotic behavior by just looking at initial values. Instead, such information is better extracted from suitable recurrence equations by looking at the characteristic polynomial and the indicial equation of the recurrence [Wimp and Zeilberger 85]. Using computer algebra, obtaining recurrence equations for the coefficient sequences is an easy task. Often, the asymptotics can be rigorously determined from a recurrence up to a constant multiple K, which cannot be determined exactly, but for which numeric approximations can be found. For instance, if $p > p_0 := (15 + 3\sqrt{33})/2$, we have

$$\begin{aligned} a_n &:= \langle x^n y^n z^n w^0\rangle \\ &\quad \times T_p\Big(1/(1 - x - y - z - w \\ &\qquad + \tfrac{64}{27}(xyz + xyw + xzw + yzw))\Big) \\ &\sim K\Big(\frac{(155 + 27\sqrt{33})\,(-4p + 3\sqrt{33} - 15)^3}{3456}\Big)^n n^{-1} \end{aligned}$$

$(n \to \infty)$ for $K \gtrsim 0.291$ (Figure 1a shows $a_n/((\cdots)^n n^{-1})$ for $p = p_0 + \frac{1}{10}$, supporting the estimate for K.) This is oscillating. For $1 < p < p_0$, the asymptotic behavior turns into

$$a_n \sim K\big(1 + \tfrac{5}{3}p\big)^{3n} n^{-1} \quad (n \to \infty),$$

for $K \gtrsim 0.227$ (Figure 1b shows $a_n/((\cdots)^n n^{-1})$ for $p = p_0 - \frac{1}{10}$, supporting the estimate for K.) This is not oscillating, but ultimately positive. This supports the conjecture $p_{\max} < p_0 \approx 16.1168$, which is little news, however, since we already know $p_{\max} < 1.66$ by inspection of initial values. Other paths to infinity that we tried do not give sharper bounds on $p_{\max}$. So it seems that $p_{\max}$ in this example is determined neither by the initial coefficients nor by the coefficients at infinity, but somehow by the coefficients "in the middle."

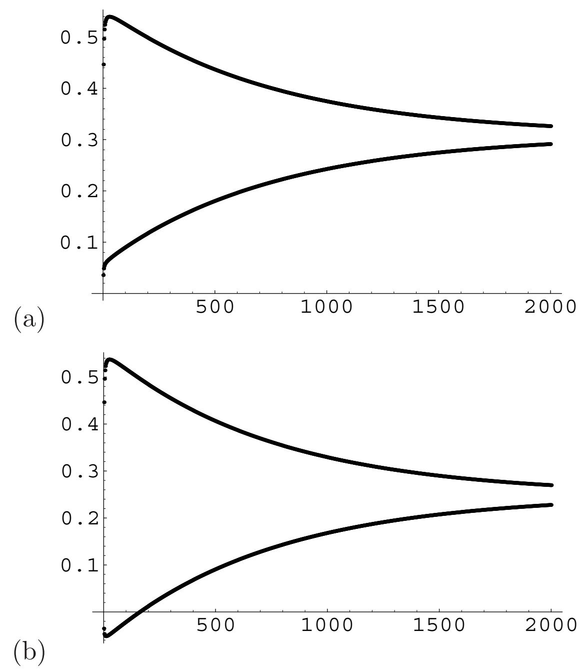

FIGURE 1. Plots for $a_n/((\ldots)n^{-1})$ supporting the asymptotic estimates given in the text.

We can consider asymptotic positivity of coefficients as an independent question that may also be asked for the rational functions considered in Empirical Results 2.1 and 2.2: what are the values $p \ge p_{\max} \ge 1$ such that the series coefficients of $T_p f$ are *ultimately* positive? Denote by $p_{\max}^{\infty}$ the supremum of these parameters. We have carried out computer experiments in search of $p_{\max}^{\infty}$, and we obtained the following empirical results.

Empirical Result 3.1. *Let $f(x, y, z) = 1/(1 - x - y - z + 4xyz)$. Then $p_{\max}^{\infty} = 2$.*

Evidence: Let $\epsilon > 0$ (sufficiently small) and $a_{n,m,k} := \langle x^n y^m z^k\rangle T_{2-\epsilon} f$.

1. First of all, we have $p_{\max}^{\infty} \le 2$, because for $\epsilon = 0$, the asymptotics on the main diagonal are

$$a_{n,n,n} \sim K(-27)^n n^{-2/3} \quad (n \to \infty)$$

with $K \gtrsim 0.25$, i.e., $a_{n,n,n}$ is ultimately oscillating for $\epsilon = 0$.

2. Let $m, k \geq 0$ be fixed and consider $a_{n,m,k}$ as a sequence in n. A direct calculation shows that

$$\begin{aligned} a_{n,m,k} &= \sum_{r=0}^{m}\sum_{t=0}^{k}\sum_{s=0}^{t}(-1)^{r+s}\binom{n}{r}\binom{n+m-r}{m-r} \\ &\quad \times \binom{n+m-2r}{s}\binom{n+m-r+t-s}{t-s} \\ &\quad \times \binom{r}{k-t}(3-\epsilon)^{r+k-t+s}(3-2\epsilon)^{k-t} \\ &\quad \times (\epsilon-1)^{r-k+t+s} \\ &= \frac{(2-\epsilon)^{2(m+k)}}{m!k!}n^{m+k} + o(n^{m+k}) \quad (n\to\infty), \end{aligned}$$

which is positive for $n \to \infty$.

3. For arbitrary (symbolic) $i \geq 0$ and the particular values $0 \leq j \leq 3$, the sequence $a_{n,n+i,j}$ satisfies a recurrence equation of order 3 that gives rise to

$$a_{n,n+i,j} \sim K(3-\epsilon)^{2n}n^{-1/2} \quad (n \to \infty)$$

for some constants K depending on i, j, and ϵ. Numeric computations suggest that these constants are positive, and hence $a_{n,n+i,j}$ is positive for $n \to \infty$.

4. For the particular values $0 \leq i, j \leq 2$, the sequence $a_{n,n+i,n+j}$ satisfies a recurrence equation of order 3 that gives rise to

$$a_{n,n+i,n+j} \sim K(3-\epsilon)^{3n}n^{-1} \quad (n \to \infty)$$

for some constants K depending on i, j, and ϵ. Numeric computations suggest that these constants are positive, and hence $a_{n,n+i,n+j}$ is positive for $n \to \infty$.

□

In parts 3 and 4, we could not carry out the arguments for both i and j generic. We did find a recurrence equation of order 6 for $a_{n,n+i,n+j}$ for generic i, j, with polynomial coefficients of total degree 16 with respect to n, i, j, but this recurrence was much too big for further processing.

Empirical Result 3.2. *Let $f(x, y, z, w) = 1/(1 - x - y - z - w + \frac{2}{3}(xy + xz + xw + yz + yw + zw))$. Then $p_{\max}^{\infty} = 3$.*

Evidence: Let $p \geq 1$ and $a_{n,m,k,l} := \langle x^n y^m z^k w^l \rangle T_p f$.

1. First of all, we have $p_{\max}^{\infty} \leq 3$, because for $p > 3$, the asymptotics on the main diagonal are determined by the two complex conjugate roots

$$\frac{9 + 30p^2 - 7p^4 \pm 4p(p^2+3)\sqrt{6-2p^2}}{9}.$$

Their modulus is $(p^2-1)^2$. Since $(p^2-1)^2$ itself is not a characteristic root, it follows [Gerhold 05] that $a_{n,n,n,n}$ is ultimately oscillating for $p > 3$.

2. For $i, j, k \geq 0$ fixed, $a_{n,i,j,k}$ is a polynomial in n of degree $i + j + k + 1$ whose leading coefficient is $p^{2(i+j+k)}/(3^{i+j+k} \cdot i! \cdot j! \cdot k!)$. Therefore $a_{n,i,j,k}$ is positive for $n \to \infty$ regardless of p.

3. For the particular values $i = 0$, 1, and $0 \leq j, k \leq 2$, the sequence $a_{n,n+i,j,k}$ satisfies a recurrence equation of order 3 that gives rise to

$$a_{n,n+i,j,k} \sim K\frac{(p+\sqrt{3})^{2n}}{3^n}n^{j+k-\frac{1}{2}} \quad (n \to \infty)$$

for some constants K depending on i, j, k, and p. Numeric computations suggest that these constants are positive, and hence $a_{n,n+i,j,k}$ is positive for $n \to \infty$ regardless of p.

4. For the particular values $0 \leq j, k \leq 1$, the sequence $a_{n,n,n+j,k}$ satisfies a recurrence equation of order 4 that gives rise to

$$a_{n,n,n+j,k} \sim K(1+p)^{3n}n^{-1} \quad (n \to \infty)$$

for some constants K depending on j, k, and p. Numeric computations suggest that these constants are positive, and hence $a_{n,n,n+j,k}$ is positive for $n \to \infty$ regardless of p.

5. The main diagonal $a_{n,n,n,n}$ satisfies a recurrence of order 4 that gives rise to

$$\begin{aligned} &a_{n,n,n,n} \\ &\quad \sim K\Big(64 + \tfrac{1}{27}(p^2-9)(2p^4 + 9p^2 + 189 \\ &\qquad - 2(p^2+3)^{3/2}p)\Big)^n n^{-3/2} \end{aligned}$$

for some constant K depending on p.

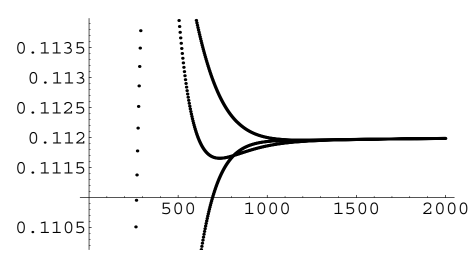

FIGURE 2. Plot for $a_{n,n,n,n}/((\ldots)n^{-3/2})$ supporting the asymptotic estimate given in the text.

Numeric computations suggest that K is positive for $p < 3$. For example, Figure 2 shows the quotients $a_{n,n,n,n}/((\cdots)^n n^{-3/2})$ for $p = 3 - \frac{1}{100}$.

$\square$

Stronger evidence in support of the conjectures made in this paper is currently beyond our computational and methodological capabilities. So are rigorous proofs.

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Manuel Kauers, Research Institute for Symbolic Computation, J. Kepler University Linz, Austria (mkauers@risc.uni-linz.ac.at)

Doron Zeilberger, Rutgers University, Piscataway, New Jersey, USA (zeilberg@math.rutgers.edu)

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