Positivity of Szegö's rational function

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Abstract

We consider the problem of deciding whether a given rational function has a power series expansion with all its coefficients positive. Introducing an elementary transformation that preserves such positivity we are able to provide an elementary proof for the positivity of Szegö's function

$$\frac{1}{(1-x)(1-y)+(1-y)(1-z)+(1-z)(1-x)}$$

which has been at the historical root of this subject starting with Szegö. We then demonstrate how to apply the transformation to prove a 4-dimensional generalization of the above function, and close with discussing the set of parameters (a, b) such that

$$\frac{1}{1-(x+y+z)+a\,(x\,y+y\,z+z\,x)+b\,x\,y\,z}$$

has positive coefficients.

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1 Introduction

A rational function is called *positive* if all its Taylor coefficients are positive. In 1930 H. Lewy and K. Friedrichs conjectured the positivity of the rational function

$$\frac{1}{(1-x)(1-y)+(1-y)(1-z)+(1-z)(1-x)}=\sum_{k,m,n\geqslant 0} a(k,m,n)\,x^k\,y^m\,z^n. \tag{1}$$

The positivity of the $a(k, m, n)$ was proved shortly after by G. Szegö employing heavy machinery in [10], but he remarks himself "die angewendeten Hilfsmittel stehen allerdings in keinem Verhältnis zu der Einfachheit des Satzes"[1]. Motivated by these words, T. Kaluza gave an elementary but technically difficult proof that was published in the very same journal [7]. R. Askey and G. Gasper also proved the above positivity in [2] using some of Szegö's observations but avoiding the use of Bessel functions in favour of Legendre polynomials. The problem has also been considered in the recent paper [8] by M. Kauers from the viewpoint of computer algebra, and Kauers establishes the result under the constraint that $k \leqslant 16$ by finding appropriate recurrences. We provide an elementary proof of Szegö's result with the main ingredient being a simple positivity preserving operation in the spirit of [5], whence we reduce the positivity of the coefficients $a(k, m, n)$ to the positivity of another rational function that is easier to handle. While our proof is indeed elementary, to check that the latter rational function is positive is most conveniently done with the aid of computer algebra.

1. "the used tools, however, are disproportionate to the simplicity of the statement"

2 Positivity preserving operations

The following elementary proposition is closely related to the positivity preserving operations given by J. Gillis, B. Reznick and D. Zeilberger in [5, Proposition 2].

Proposition 1. *Fix $n \geqslant 1$. Let $1 \leqslant j \leqslant n$ and suppose that the polynomial $p(x_1, \ldots, x_n)$ is linear in x_j. If $1/p(x_1, \ldots, x_n)$ is positive then so is*

$$T_{j,\lambda}\left(\frac{1}{p(x_1, \ldots, x_n)}\right) := \frac{1}{p(x_1, \ldots, x_n) - \lambda\, x_j\, p(x_1, \ldots, x_{j-1}, 0, x_{j+1}, \ldots, x_n)}$$

whenever $\lambda \geqslant 0$. In other words, the operator $T_{j,\lambda}$ as defined above is positivity preserving for $\lambda \geqslant 0$.

Proof. We may assume $j = 1$. Write $p(x_1, \ldots, x_n) = a(x_2, \ldots, x_n) - x_1\, b(x_2, \ldots, x_n)$. Since

$$\frac{1}{p} = \frac{1}{a - x_1\, b} = \sum_{n \geqslant 0} \frac{b^n}{a^{n+1}}\, x_1^n$$

has positive coefficients so does b^n / a^{n+1}. The quotient

$$\frac{b^n}{a^{n+1}} \frac{x_1^n}{(1 - \lambda x_1)^{n+1}}$$

has nonnegative coefficients, and for $n = 0$ they are all positive. This finally implies the positivity of

$$\sum_{n \geqslant 0} \frac{(x_1 b)^n}{((1 - \lambda x_1) a)^{n+1}} = \frac{1}{(1 - \lambda x_1)\, a - x_1 b} = \frac{1}{p - \lambda x_1 a}. \qquad \square$$

In this paper, we will only be interested in the positivity of symmetric rational functions $1/p$. We therefore introduce another operator which preserves both positivity and symmetry.

Corollary 1. *The operator T_λ defined by*

$$T_\lambda := T_{n,\lambda} \cdots T_{2,\lambda} T_{1,\lambda}$$

is positivity preserving for $\lambda \geqslant 0$.

Note that $T_\lambda(1/p)$ is only defined for polynomials p which are linear in each of their variables. Further note that $T_{j,\lambda}$ is invertible with $T_{j,\lambda}^{-1} = T_{j,-\lambda}$. Since the operators $T_{1,\lambda}, T_{2,\lambda}, \ldots, T_{n,\lambda}$ commute, this shows that T_λ is invertible as well and $T_\lambda^{-1} = T_{-\lambda}$. Hence, in order to establish the positivity of $1/p$ it is sufficient to do so for some $T_{-\lambda}(1/p)$ with $\lambda \geqslant 0$. That T_λ preserves symmetry also follows from the fact that $T_{1,\lambda}, \ldots, T_{n,\lambda}$ commute.

Example 1. To prove positivity of $1/p(x, y, z)$, assuming p to be linear in each of x, y, z, it suffices to prove positivity of

$$T_{-1}\left(\frac{1}{p(x, y, z)}\right) = \begin{array}{l}(p(x, y, z) + x\, p(0, y, z) + y\, p(x, 0, z) + z\, p(x, y, 0) \\ \quad + x\, y\, p(0, 0, z) + y\, z\, p(x, 0, 0) + z\, x\, p(0, y, 0) + x\, y\, z\, p(0, 0, 0))^{-1}\end{array}$$

Notice that the right-hand side is indeed a symmetric rational function if p is symmetric itself.

3 Szegö's rational function

3.1 Positivity of Szegö's rational function

Theorem 1. *Szegö's rational function*

$$f(x,y,z) := \frac{1}{1-2\,(x+y+z)+3\,(x\,y+y\,z+z\,x)}$$

is positive.

Remark 1. Note that up to rescaling this is the rational function from (1), namely

$$\frac{1}{3}\,f\Big(\frac{x}{3},\frac{y}{3},\frac{z}{3}\Big) = \frac{1}{(1-x)(1-y)+(1-y)(1-z)+(1-z)(1-x)}.$$

Proof. The denominator of f is linear in all the variables x, y, z, so we can apply our inverted positivity preserving operation T_{-1}. We obtain

$$g(x,y,z) := T_{-1}(f(x,y,z)) = \frac{1}{1-(x+y+z)+4\,x\,y\,z}.$$

By Corollary 1 positivity of g implies positivity of f. The positivity of g, however, is well-known, and several short proofs have been given in the literature (not so, to our knowledge, for f). One possibility is to note that the coefficients $b(k,\,m,\,n)$ of g satisfy the following recurrence, first observed by J. Gillis and J. Kleeman [4],

$$(1+n)\,b(k+1,m+1,n+1) = 2\,(n+m-k)\,b(k+1,m,n) + (1+n-m+k)\,b(k+1,m+1,n),$$

which together with the initial $b(0,\,0,\,0)=1$ proves positivity of the $b(k,\,m,\,n)$ by induction. That the $b(k,\,m,\,n)$ satisfy this recurrence is verified by just checking that their generating function g solves the corresponding differential equation. □

Remark 2. Kauers describes in [8] how to automatically find positivity proving recurrences with computer algebra, and also remarks that no such first-order recurrence with linear coefficients exists for Szegö's f.

Another simple proof of the positivity of g based on MacMahon's master theorem is given by M. Ismail and M. Tamhankar in [6]. We will discuss this theorem in Section 3.3. The reason for doing so is that we discovered the transformation presented in Corollary 1 by applying MacMahon's master theorem, whence it is possible to just *see* its impact.

3.2 A 4-dimensional generalization

Following [10, §3] we define

$$q_n(t) = \prod_{k=1}^{n}\,(t-x_k),$$

and observe that one can recover Szegö's function as

$$\frac{1}{q_3'(1)} = \frac{1}{(1-x_1)(1-x_2)+(1-x_2)(1-x_3)+(1-x_3)(1-x_1)}.$$

Szegö proves that $1/q_n'(1)$ as a rational function in $x_1, \ldots, x_n$ has positive Taylor coefficients for all $n \geqslant 2$, and remarks that the essential difficulty lies in the cases $n=3$ and $n=4$. While our previous discussion covers $n=3$, we now want to briefly demonstrate how to use the operators T_λ from Corollary 1 to also establish the case $n=4$ in an elementary way.

Theorem 2. *The rational function*

$$\frac{1}{q_4'(1)} = \frac{1}{\sum_{i<j<k}(1-x_i)(1-x_j)(1-x_k)},$$

where $i, j, k = 1, 2, 3, 4,$ is positive.

Proof. Expanding the denominator of $1/q_4'(1)$ and rescaling produces the rational function

$$\frac{1}{1-3\sum_i x_i + 8\sum_{i<j} x_i x_j - 16\sum_{i<j<k} x_i x_j x_k}.$$

Applying T_{-2} we find that it suffices to establish positivity of

$$\frac{1}{1-\sum_i x_i + 4\sum_{i<j<k} x_i x_j x_k - 16\, x_1 x_2 x_3 x_4}.$$

This again is a well-known result. In particular, Gillis, Reznick and Zeilberger demonstrate in [5] how a single application of their elementary methods can be used to deduce the desired positivity. □

For other possible generalizations of Szegö's function the interested reader is referred to [2], [1]. In [3] relations to rearrangement problems and integrals of products of Laguerre polynomials are studied.

3.3 MacMahon's master theorem

The following is a celebrated result of P. A. MacMahon published in [9], and coined by himself as "a master theorem in the Theory of Permutations".

Theorem 3. (MacMahon, 1915) *Let R be a commutative ring, $A \in R^{n\times n}$ a matrix, and $x = (x_1, \ldots, x_n)$ commuting indeterminants. For every multi-index $m = (m_1, \ldots, m_n) \in \mathbb{Z}^n_{\geqslant 0}$*

$$[x^m] \prod_{i=1}^{n} \left(\sum_{j=1}^{n} A_{i,j} x_i \right)^{m_i} = [x^m] \det\left(I_n - A \begin{pmatrix} x_1 & & \\ & \ddots & \\ & & x_n \end{pmatrix} \right)^{-1},$$

where $[x^m]$ denotes the coefficient of $x_1^{m_1} \cdots x_n^{m_n}$ in the expansion of what follows.

We find, preferably by using computer algebra, that Szegö's function $f(x, y, z)$ can be expressed as

$$\frac{1}{1-2(x+y+z)+3(xy+yz+zx)} = \det\left(I_3 - \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}\begin{pmatrix} x & & \\ & y & \\ & & z \end{pmatrix}\right)^{-1}.$$

MacMahon's theorem 3 now asserts that the coefficient $a(k, m, n)$ of $x^k y^m z^n$ in this expansion is equal to the coefficient of $x^k y^m z^n$ in

$$(2x-y-z)^k(-x+2y-z)^m(-x-y+2z)^n.$$

Using the binomial theorem this product is equal to

$$\sum_{r,s,t} \binom{k}{r}\binom{m}{s}\binom{n}{t} x^{k-r} y^{m-s} z^{n-t} (x-y-z)^r(-x+y-z)^s(-x-y+z)^t,$$

which shows that in order to establish positivity of the $a(k, m, n)$ it is sufficient to prove positivity of the coefficient of $x^r y^s z^t$ in

$$(x-y-z)^r(-x+y-z)^s(-x-y+z)^t.$$

By applying MacMahon's master theorem 3 backwards we find that

$$\det\left(I_3 - \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}\begin{pmatrix} x & & \\ & y & \\ & & z \end{pmatrix}\right)^{-1} = \frac{1}{1-(x+y+z)+4xyz},$$

which once more reduces positivity of f to the positivity of g.

With this example in mind, we see the following relation to the positivity preserving operations T_λ: Let f be a rational function that T_λ can be applied to and which can be represented as $f = 1/\det(I - AX)$ for some matrix A (here X denotes the diagonal matrix with the variables of f as its entries). Then $T_\lambda(f) = 1/\det(I - A_\lambda X)$ where A_λ is obtained from A by increasing all its diagonal entries by λ. Similarly, application of $T_{j,\lambda}$ corresponds to increasing the j-th diagonal element by λ. Thus when working with a matrix A corresponding to f instead of with f itself, the action of the positivity preserving operators described here is plainly visible.

4 On positivity of a family of rational functions

Kauers states that "it is easy to show that there can be no algorithm which for a given multivariate rational function decides whether all its series coefficients are positive", see [8]. Therefore we focus on the reciprocals of certain symmetric polynomials. In the 3-dimensional case we have the 4 elementary symmetric polynomials

$$1, \quad x+y+z, \quad xy+yz+zx, \quad xyz,$$

and if we further require that every variable appears at most linearly, the most general normalized candidate for positivity is

$$h_{a,b}(x,y,z)=\frac{1}{1-(x+y+z)+a\,(x\,y+y\,z+z\,x)+b\,x\,y\,z}.$$

We are interested in the set of all (a,b) such that $h_{a,b}$ has positive coefficients. First, we note that positivity of some $h_{a,b}$ implies positivity of $h_{a',b'}$ whenever $a'\leqslant a$ and $b'\leqslant b$. This is a consequence of the following general fact.

Proposition 2. *Let $1/p(x_1,\ldots,x_r)$ be a positive rational function, and $q(x_1,\ldots,x_r)$ any polynomial with non-negative coefficients. Then the rational function*

$$\frac{1}{p-q}$$

is positive provided that it has no pole at the origin.

Proof. This follows from the geometric summation

$$\frac{1}{p-q}=\frac{1}{p}\sum_{n\geqslant 0}\left(\frac{q}{p}\right)^n. \qquad \square$$

Example 2. We shortly demonstrate another application of this fact. In [8], it was conjectured that the rational function

$$\frac{1}{1-(x+y+z)+\frac{1}{4}\,(x^2+y^2+z^2)}$$

is positive. Clearly,

$$\frac{1}{(1-x)^2}$$

has positive coefficents, and thus has

$$\frac{1}{(1-\frac{x+y+z}{2})^2}=\frac{1}{1-(x+y+z)+\frac{1}{2}\,(x\,y+y\,z+z\,x)+\frac{1}{4}\,(x^2+y^2+z^2)}.$$

Proposition 2 now implies positivity of the function considered by Kauers.

Based upon numerical evidence and partial proofs, which will be provided in the sequel, we present the following conjecture attempting to describe the set of all (a,b) such that $h_{a,b}$ has positive coefficients.

Conjecture 1. *The rational function $h_{a,b}$ has positive coefficients if and only if*

$$\begin{cases} b<6(1-a)\\ b\leqslant 2-3a+2(1-a)^{3/2}\\ a\leqslant 1\end{cases}.$$

Figure 1 shows the region defined by the restrictions given in Conjecture 1 with the points corresponding to Szegö's function $f(x,y,z)=h_{3/4,0}(2x,2y,2z)$ and $g=h_{0,4}$ marked.

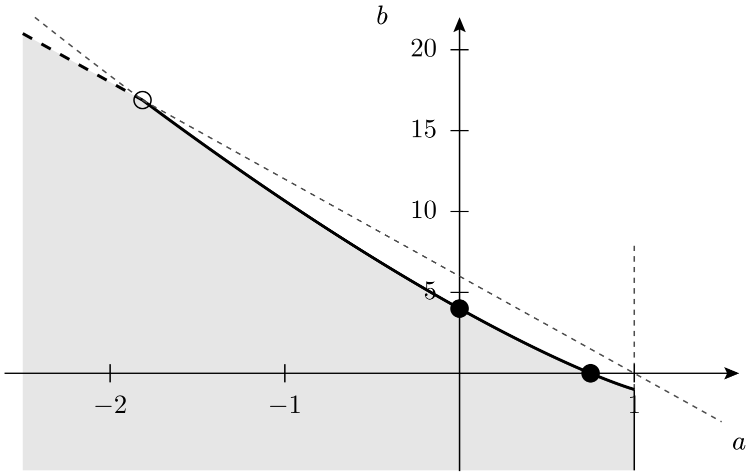

Figure 1. Region of Positivity of $h_{a,b}$

First, we turn to the "if" part of Conjecture 1, that is conditions for the (a, b) that are sufficient for positivity of $h_{a,b}$.

Proposition 3. *$h_{a,b}$ is positive if $0\leqslant a\leqslant 1$ and $b\leqslant 2-3a+2(1-a)^{3/2}$.*

Proof. Let $\lambda\geqslant 0$. By Corollary 1 positivity of some $h_{a,b}$ implies positivity of $h_{a',b'}:=T_\lambda(h_{a,b})$ (here we mean that $h_{a',b'}$ equals $T_\lambda(h_{a,b})$ up to rescaling the variables), where

$$a'=\frac{a+2\lambda+\lambda^2}{(1+\lambda)^2},\quad b'=\frac{b-3\lambda a-3\lambda^2-\lambda^3}{(1+\lambda)^3}.$$

Starting with the positivity of $g=h_{0,4}$, that is $(a,b)=(0,4)$, we find that $b'=2-3a'+2(1-a')^{3/2}$. Using Proposition 2 this proves the case $0\leqslant a<1$. For $a=1$ observe that

$$h_{1,-1}(x,y,z)=\frac{1}{(1-x)(1-y)(1-z)}$$

is obviously positive. □

Using the positivity of g and the positivity preserving operations T_λ we have thus been able to prove the "if" part of Conjecture 1 under the hypothesis that $a\geqslant 0$. Clearly, we can strengthen this hypothesis to $a\geqslant a_1$ if we succeed in proving the positivity of h_{a_1,b_1} with $b_1=2-3a_1+2(1-a_1)^{3/2}$. However, according to Conjecture 1 we neccessarily have $a_1>a_0$, where $a_0\approx-1.81451$ is the unique real solution of

$$2-3a_0+2(1-a_0)^{3/2}=6(1-a_0).$$

Let's now consider the "only if" direction of Conjecture 1.

Proposition 4. *$h_{a,b}$ is positive only if $b < 6(1-a)$ and $a \leqslant 1$.*

Proof. Observe that the coefficient of $x\,y\,z$ in the expansion of $h_{a,b}(x,y,z)$ evaluates as $6(1-a)-b$ which proves that $b<6(1-a)$ for positivity.

For the second claim we expand $h_{a,b}(x,y,0)$ as

$$h_{a,b}(x,y,0)=\frac{1}{1-x-y+a\,x\,y}=\sum_{n\geqslant 0}\frac{(1-a\,x)^n}{(1-x)^{n+1}}\,y^n.$$

Using

$$\frac{1}{(1-x)^{n+1}}=\sum_{m\geqslant 0}\binom{n+m}{n}x^m,$$

we deduce that the coefficient of $x\,y^n$ in $h_{a,b}(x,y,z)$ is given by $n+1-n\,a$. Positivity of $h_{a,b}$ thus implies that

$$a<\frac{n+1}{n}$$

for all positive integers n. □

Proposition 3 is based upon the positivity of $g=h_{0,4}$, which by Proposition 2 implies that $b\leqslant 4$ suffices for positivity of $h_{0,b}$. This bound turns out to be sharp.

Proposition 5. *$h_{0,b}$ is positive only if $b\leqslant 4$.*

Proof. We expand $h_{0,b}$ as

$$h_{0,b}(x,y,z)=\frac{1}{1-x-y-z+b\,x\,y\,z}=\sum_{n\geqslant 0}\frac{(1-b\,x\,y)^n}{(1-x-y)^{n+1}}\,z^n.$$

Using

$$\frac{1}{(1-x-y)^{n+1}}=\sum_{m\geqslant 0}\binom{n+m}{n}(x+y)^m,$$

we conclude that the coefficient of $x\,y^n\,z^n$ in $h_{0,b}(x,y,z)$ is given by

$$(n+1)\binom{2n+1}{n}-b\,n\binom{2n-1}{n}.$$

Positivity of $h_{0,b}$ then implies that

$$b<\frac{2\,(2n+1)}{n}$$

for all integers $n>0$. □

Corollary 2. *Let $a\leqslant 0$. Then $h_{a,b}$ is positive only if $b\leqslant 2-3a+2(1-a)^{3/2}$.*

Proof. Otherwise an application of T_λ with appropriate $\lambda>0$ would produce (after normalization) a positive $h_{0,b'}$ with $b'>4$ contradicting Proposition 5. □

To improve on the hypothesis $a \leqslant 0$, it would be desirable to show optimality of Szegö's function, that is that $h_{a,0}$ is positive only if $a \leqslant 3/4$. As in the proof of Proposition 5 we believe that it suffices to consider the coefficients of $x\, y^n\, z^n$ in $h_{a,0}(x, y, z)$. While we readily find a second order recurrence for those coefficients we didn't see how to derive the necessity of $a \leqslant 3/4$ in order to prove positivity.

Example 3. By computing the first 100 coefficients of $x\, y^n\, z^n$ in $h_{a,0}(x, y, z)$ we learn that $h_{a,0}$ is positive only if $a < 0.75188$.

The (conjectured) optimality of Szegö's function f is surprising in this context since $f = T_1(g)$ allows us to conclude the positivity of f from the positivity of g but not vice versa. Yet, the positivity preserving operator T_1 still provided us with an optimal result. In fact, more seems to be true. As stated in Conjecture 1, starting with a positive $h_{a,b}$ which is optimal (in the sense that increasing either a or b will destroy positivity) the positivity preserving operators T_λ, $\lambda \geqslant 0$, not only yield a positive rational function $T_\lambda(h_{a,b})$ but again they seem to produce an optimal rational function.

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