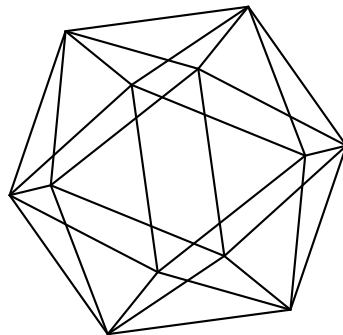


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POSITIVITY OF RATIONAL FUNCTIONS AND THEIR DIAGONALS

ARMIN STRAUB AND WADIM ZUDILIN

*To Dick Askey on the occasion of his birthday,
with many positive wishes*

ABSTRACT. The problem to decide whether a given rational function in several variables is positive, in the sense that all its Taylor coefficients are positive, goes back to Szegő as well as Askey and Gasper, who inspired more recent work. It is well known that the diagonal coefficients of rational functions are D -finite. This note is motivated by the observation that, for several of the rational functions whose positivity has received special attention, the diagonal terms in fact have arithmetic significance and arise from differential equations that have modular parametrization. In each of these cases, this allows us to conclude that the diagonal is positive.

Further inspired by a result of Gillis, Reznick and Zeilberger, we investigate the relation between positivity of a rational function and the positivity of its diagonal.

1. INTRODUCTION

The question to decide whether a given rational function is *positive*, that is, whether its Taylor coefficients are all positive, goes back to Szegő [22] and has since been investigated by many authors including Askey and Gasper [2, 3, 4], Koornwinder [14], Ismail and Tamhankar [11], Gillis, Reznick and Zeilberger [10], Kauers [12], Straub [21], Kauers and Zeilberger [13], Scott and Sokal [20]. The interested reader will find a nice historical account in [20]. A particularly interesting instance is the Askey–Gasper rational function

$$(1) \quad A(x, y, z) := \frac{1}{1 - x - y - z + 4xyz},$$

whose positivity is proved in [4] and [10]. Generalizations to more than three variables are rarely tractable, with the longstanding conjecture of the positivity of

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

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also referred to as the Lewy–Askey problem. Very recently, Scott and Sokal [20] succeeded in proving the non-negativity of (2), both in an elementary way and based on more general results on the basis generating polynomials of certain classes of matroids. Note that by a result from [13] the positivity of (2) would follow from the positivity of

$$D(x, z, y, w) := \frac{1}{1 - x - y - z - w + 2(yzw + xzw + xyw + xyz) + 4xyzw}.$$

In another direction, Gillis, Reznick and Zeilberger conjecture in [10] that

$$(3) \quad \frac{1}{1 - (x_1 + x_2 + \dots + x_d) + d!x_1x_2 \cdots x_d}$$

has non-negative coefficients for any $d \geq 4$. It is further shown (though the proof is *omitted due to its length*) that, in order to show the non-negativity of the rational functions in (3), it suffices to prove that their *diagonal* Taylor coefficients are non-negative. Based on this claim, the cases $d = 4, 5, 6$ were established by Kauers [12], who found and examined recurrences for the respective diagonal coefficients.

The above claim from [10] suggests the following question. Here, we denote by $e_k(x_1, \dots, x_d)$ the elementary symmetric polynomials defined by

$$(4) \quad \prod_{j=1}^d (x + x_j) = \sum_{k=0}^d e_k(x_1, \dots, x_d) x^{d-k}.$$

Question 1.1. Under what (natural) condition(s) is the positivity of a rational function $h(x_1, \dots, x_d)$ of the form

$$(5) \quad h(x_1, \dots, x_d) = \frac{1}{\sum_{k=0}^d c_k e_k(x_1, \dots, x_d)}$$

implied by the positivity of its diagonal?

For example, would the positivity of $h(x_1, \dots, x_{d-1}, 0)$ be a sufficient condition?

Another motivation for this question is the fact that for several important rational functions, like the ones reproduced above, the diagonal coefficients are arithmetically interesting sequences. In particular, expressing them in terms of known hypergeometric summations sometimes makes their positivity apparent. For instance, the diagonal sequence for $A(x, y, z)$ is

$$(6) \quad a_{n,n,n} = \sum_{k=0}^n \binom{n}{k}^3,$$

see Example 3.4, while the diagonal of $D(x, y, z, w)$ is given by

$$d_{n,n,n,n} = \sum_{k=0}^n \binom{n}{k}^2 \binom{2k}{n},$$

as is shown in Example 4.2. Since these diagonal sequences are manifestly positive, sufficient progress on Question 1.1 might provide a proof of the conjectured positivity of $D(x, y, z, w)$. More generally, proving positivity of a single sequence is much simpler from a practical point of view than proving positivity of all Taylor coefficients of a rational function, and tools such as cylindrical algebraic decomposition can be used for this task rather successfully in specific examples, as illustrated by [12] and observed in some of the examples herein.

We note that, with no loss of generality, we may assume in Question 1.1 that $c_0 = 1$.

In Section 2, we answer Question 1.1 in the affirmative when $d = 2$. The three and four-dimensional cases are discussed in Sections 3 and 4, while Section 5 covers an approach to positivity via asymptotics. In particular, we prove that the conjectural conditions, given in [21], for positivity of rational functions in three variables are indeed necessary.

2. THE TWO-DIMENSIONAL CASE

In the case of only two variables, we are thus interested in the rational function

$$h(x, y) = \frac{1}{1 + c_1(x + y) + c_2xy}.$$

Note that the condition $c_1 < 0$ is necessary to ensure the positivity of $h(x, y)$, as $-c_1$ is a Taylor coefficient of its series expansion. Our next example demonstrates that this condition is not implied by the positivity of the diagonal of $h(x, y)$.

Example 2.1. The rational function $1/(1 + x + y)$ has positive diagonal coefficients but is not positive. This illustrates that some condition is indeed needed in Question 1.1.

Theorem 2.2. *A two-variable rational function*

$$h(x, y) = \frac{1}{1 + c_1(x + y) + c_2xy}$$

is positive, if both $h(x, 0)$ and the diagonal of $h(x, y)$ are positive.

Proof. The positivity of $h(x, 0)$ implies that $c_1 < 0$. Upon rescaling the variables by a positive factor, we may assume that $c_1 = -1$ and write our rational function in the form

$$(7) \quad \frac{1}{1 - (x + y) + axy} = \sum_{n,m=0}^{\infty} a_{n,m}x^n y^m.$$

As demonstrated in the course of [21, Proposition 4], this rational function is positive if and only if $a \leq 1$. On the other hand, the diagonal terms

$a_n := a_{n,n}$ of the Taylor expansion are given by

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

We observe that the sequence a_n is characterized by the generating series

$$\sum_{n=0}^{\infty} a_n z^n = \frac{1}{\sqrt{1 - 2(2-a)z + a^2 z^2}}.$$

For $a > 1$, the quadratic polynomial $1 - 2(2-a)z + a^2 z^2$ has non-real roots, from which we conclude that a_n is (eventually) sign-indefinite. Therefore, the series (7) is positive if and only if its diagonal terms are positive. \square

Theorem 2.2 answers Question 1.1 in the affirmative when $d = 2$.

Remark 2.3. The sequence a_n satisfies the three-term recurrence

$$(n+1)a_{n+1} = (2-a)(2n+1)a_n - a^2 n a_{n-1},$$

which has characteristic polynomial $(x+a)^2 - 4x$. Note that, for $a > 1$, this polynomial has complex roots.

The ultimate reduction to $d = 1$ and $d = 2$ performed in this section shows that for $d \geq 3$ we can normalize, without loss of generality, our d -variable rational function (5) to satisfy $c_0 = 1$, $c_1 = -1$ and also $c_2 = a \leq 1$. This will be the canonical form of a rational function in Question 1.1.

3. THE THREE-DIMENSIONAL CASE

A partially conjectural classification of positive rational functions of the form

$$(8) \quad h_{a,b}(x, y, z) = \frac{1}{1 - (x + y + z) + a(xy + yz + zx) + bxyz}$$

has been given in [21]. It is conjectured there [21, Conjecture 1] that $h_{a,b}$ is positive if and only if the three inequalities $a \leq 1$, $b < 6(1-a)$, $b \leq 2 - 3a + 2(1-a)^{3/2}$ hold. In Theorem 5.7 below we show that all three conditions are indeed necessary for positivity.

Example 3.1. It is proven in [21] that the rational function $h_{a,b}$ with

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

is positive for all $\lambda \geq 0$. The conjecture mentioned above predicts that it is, in fact, positive as long as $\lambda > (1 + \sqrt{2})^{1/3} - (1 + \sqrt{2})^{-1/3} - 1 \approx -0.403928$. Note that this rational function, after a scaling of variables, is

$$\frac{1}{1 - (\lambda+1)(x+y+z) + \lambda(\lambda+2)(xy+yz+zx) - (\lambda-1)(\lambda+2)^2 xyz}.$$

It appears that the Taylor coefficients of this rational function are polynomials in λ with positive coefficients.

Note that, by the results of Section 2, $h_{a,b}(x, y, 0)$ is positive if and only if $a \leq 1$. The next conjecture is therefore equivalent to an affirmative answer to Question 1.1 for $d = 3$.

Conjecture 3.2. *Suppose that $a \leq 1$. Then the rational function (8) is positive if and only if its diagonal is positive.*

In the case $a > 1$, which is not covered by Conjecture 3.2, the following is a conjectural characterization of the rational functions which have positive diagonal coefficients.

Conjecture 3.3. *Let $a \geq 1$. The diagonal of (8) is positive if and only if $b \leq -a^3$.*

That the case $b = -a^3$ plays a special role can be seen from the characteristic polynomial of the recurrence of minimal order for the diagonal coefficients. Namely, the diagonal coefficients a_n of $h_{a,b}$, as defined in (8), satisfy a fourth order recurrence (the coefficients have degree 4 in n , degree 9 in a and degree 5 in b), whose characteristic polynomial is

$$(9) \quad (a^3 + b)(a^3 + ab - (1 - a)x)((x + b)^3 + 27x(a^3 + ab - (1 - a)x)).$$

Obviously, the first factor vanishes when $b = -a^3$. We further observe that the cubic factor in (9) has discriminant

$$-3^9(a^3 - 3a^2 - b)^2(4a^3 - 3a^2 + 6ab + b^2 - 4b).$$

The second factor vanishes if and only if $b = 2 - 3a \pm 2(1 - a)^{3/2}$, which includes the principal condition of [21, Conjecture 1] as stated at the beginning of this section; see also Example 5.2.

In the remainder of this section, we consider two cases of particular interest in the three-variable case, namely the Askey–Gasper rational function $A(x, y, z)$ from (1) as well as Szegő’s rational function

$$(10) \quad S(x, y, z) = \frac{1}{1 - (x + y + z) + \frac{3}{4}(xy + yz + zx)}.$$

In both cases, we exhibit the arithmetic nature of the diagonals and demonstrate that positivity follows as a consequence.

Example 3.4. According to [8], the diagonal sequence $a_n := a_{n,n,n}$ for $A(x, y, z)$ as in (1) satisfies the three-term recurrence equation

$$(n + 1)^2 a_{n+1} = (7n^2 + 7n + 2)a_n + 8n^2 a_{n-1}.$$

The same recursion holds for the sequence $a_n = \sum_{k=0}^n \binom{n}{k}^3$, also known as Franel numbers, which is a classical result of Franel [9]. As indicated in (6), the diagonal of $A(x, y, z)$ is thus given by the Franel numbers. The sequence a_n is an Apéry-like sequence, namely [1, sequence (4.8) (a)], and the (Calabi–Yau) differential equation satisfied by the generating function

has modular parametrization. As a consequence, the generating function has a hypergeometric form, namely

$$(11) \quad \sum_{n=0}^{\infty} a_n z^n = \frac{1}{1-2z} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \mid \frac{27z^2}{(1-2z)^3}\right),$$

which we record for comparison with the next example. Here and in what follows

$${}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} \mid z\right) = \sum_{n=0}^{\infty} z^n \prod_{j=0}^{n-1} \frac{(a+j)(b+j)}{(1+j)(c+j)}$$

is the hypergeometric function. Note that positivity is still apparent from (11).

Example 3.5. As shown in [21], the positivity of $S(x, y, z)$ can be deduced from the positivity of $A(x, y, z)$. On the other hand, the diagonals of the two are not related to each other in an easy way; the diagonal terms $s_n = [(xyz)^n]S(2x, 2y, 2z)$ are given by

$$1, 12, 198, 3720, 75690, 1626912, \dots$$

and satisfy the recurrence

$$(12) \quad 2(n+1)^2 s_{n+1} = 3(27n^2 + 27n + 8) s_n - 81(3n-1)(3n+1) s_{n-1}.$$

Denoting by $y_0(z) = \sum_{n \geq 0} s_n z^n$ the generating function of this sequence, it is routine to verify that

$$(13) \quad y_0(z) = {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \mid 27z(2-27z)\right);$$

indeed, both sides in (13) satisfy the same differential equation. See Remark 3.7 below on how one can find this expression. We note that (13) implies the binomial formula

$$s_n = \sum_{k=0}^n (-27)^{n-k} 2^{2k-n} \frac{(3k)!}{k!^3} \binom{k}{n-k},$$

though positivity is not apparent here.

Lemma 3.6. *The sequence s_n in Example 3.5 is positive.*

Proof. To deduce positivity of $y_0(z)$ in (13), start with Ramanujan's cubic transformation [6, p. 97]

$${}_2F_1\left(\frac{1}{3}, \frac{2}{3} \mid 1 - \left(\frac{1-x}{1+2x}\right)^3\right) = (1+2x) {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \mid x^3\right),$$

which is proven in [7]; see also [15, Corollary 6.2]. With x and z related by

$$27z(2-27z) = 1 - \left(\frac{1-x}{1+2x}\right)^3,$$

we find that

$$2x(z) = \frac{3}{1 + 2(1 - 27z)^{2/3}} - 1.$$

The binomial theorem shows that $(1 - 27z)^{2/3} = 1 - zg(z)$ for some $g(z)$ with positive Taylor coefficients. It follows that $x(z) = c_1z + c_2z^2 + \dots$ for positive c_j , so that

$$y_0(z) = (1 + 2x(z))_2F_1\left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| x(z)^3\right)$$

is seen to have positive coefficients. □

Remark 3.7. Let us briefly indicate how we found (13). First, note that $y_0(z)$ is the analytical solution of the differential equation corresponding to (12) characterized by $y_0(0) = 1$. Let $y_1(z)$ be the solution such that $y_1(z) - y_0(z) \log(z) \in z\mathbb{Q}[[z]]$. Then

$$q(z) := \exp\left(\frac{y_1(z)}{y_0(z)}\right) = z + \frac{33z^2}{2} + 306z^3 + \frac{12203z^4}{2} + 128109z^5 + O(z^6).$$

Denoting by $z(q)$ the inverse function, we observed, by computing the first few terms of the q -expansion, that

$$y_0(z(q/2)) = \sum_{n,m \in \mathbb{Z}} q^{n^2 + nm + m^2}.$$

The right-hand side is the theta series of the planar hexagonal lattice, also known as the first cubic theta function $a(q)$, and its relation to the hypergeometric function in (13) is well known; see, for instance, [7]. For further background on this approach we refer the interested reader to [1].

4. EXAMPLES IN THE FOUR-DIMENSIONAL CASE

We now study positivity of the rational functions in four variables, which are of type (5). That is, we consider the rational functions

$$(14) \quad h_{a,b,c}(\mathbf{x}) = \frac{1}{1 - e_1(\mathbf{x}) + ae_2(\mathbf{x}) + be_3(\mathbf{x}) + ce_4(\mathbf{x})},$$

where $\mathbf{x} = (x_1, x_2, x_3, x_4)$ and $e_k(\mathbf{x})$ are the elementary symmetric functions defined in (4). Table 1 summarizes the examples we discuss in this section.

a	b	c	
0	2	4	conjectured in [13]
$\frac{2}{3}$	0	0	conjectured in [3]; proven in [20]; implied by $h_{0,2,4}$
0	$\frac{64}{27}$	0	conjectured in [12]
0	0	24	conjectured in [10]; proven in [12]
0	4	-16	proven in [14]; see also [10]
$\frac{8}{9}$	$-\frac{16}{27}$	0	proven in [22, §3]; implied by $h_{0,4,-16}$

TABLE 1. Interesting instances of $h_{a,b,c}$ as in (14)

Example 4.1 (Askey–Gasper rational function). In [3], Askey and Gasper mention the following four-dimensional generalization of Szegő’s function

$$h_{2/3,0,0}(x, y, z, w) = \frac{1}{1 - (x + y + z + w) + \frac{2}{3}(xy + xz + xw + yz + yw + zw)},$$

which is just a rescaled version of $1/e_2(1 - x, 1 - y, 1 - z, 1 - w)$. As already mentioned in the introduction, the non-negativity of this rational function was recently established in [20]. The scaled initial diagonal terms $s_n := 9^n[(xyzw)^n]h_{2/3,0,0}(x, y, z, w)$ are

$$1, 24, 1080, 58560, 3490200, 220739904, \dots,$$

and one checks that $s_n = \binom{2n}{n}u_n$, where the sequence u_n satisfies the recurrence equation

$$3(n + 1)^2u_{n+1} = 4(28n^2 + 28n + 9)u_n - 64(4n - 1)(4n + 1)u_{n-1}.$$

As in Example 3.5, the differential equation, of which the generating function $y_0(z) = \sum_{n \geq 0} u_n z^n$ is the unique analytical solution with value 1 at $z = 0$, admits modular parametrization. This fact was found and communicated to us by van Straten. As a consequence, we have the hypergeometric representation

(15)

$$y_0(z) = \frac{1}{(1 - 48z + 12288z^3)^{1/4}} {}_2F_1\left(\frac{1}{12}, \frac{5}{12} \mid \frac{-1728z^2(3 - 64z)(1 - 16z)^6}{(1 - 48z + 12288z^3)^3}\right),$$

which, once found, can be verified by comparing the differential equations satisfied by both sides. In fact, using hypergeometric transformations, we find that (15) simplifies to

$$(16) \quad y_0(z) = \frac{1}{\sqrt{1 - 24z}} {}_2F_1\left(\frac{1}{4}, \frac{3}{4} \mid \frac{-64z^2(3 - 64z)}{(1 - 24z)^2}\right).$$

As in Example 3.5, we can now use the arithmetic properties of this function to show that the sequence u_n , hence the diagonal terms s_n , are indeed positive. To do so, we may proceed as in Lemma 3.6, except now using Ramanujan’s quadratic transformation [6, p. 146] (also proven in [15, Corollary 6.2]). Alternatively, we can prove positivity of the diagonal terms from the above three-term recurrence using cylindrical algebraic decomposition in the style of [12].

Example 4.2 (Kauers–Zeilberger rational function). On the other hand, the positivity of the rational function in the previous example is implied, as shown in [13] using positivity preserving operators, by the positivity of the rational function

$$h_{0,2,4}(x, y, z, w) = \frac{1}{1 - (x + y + z + w) + 2e_3(x, y, z, w) + 4xyzw},$$

which we also refer to as $D(x, y, z, w)$. This rational function, as mentioned in the introduction, has particularly appealing diagonal coefficients. Namely,

expanding

$$D(x, y, z, w) = \sum_{n=0}^{\infty} [(x + y + z + w) - 2(yzw + xzw + xyw + xyz) - 4xyzw]^n,$$

and applying the binomial theorem, one obtains a five-fold sum for the diagonal coefficients $d_n = d_{n,n,n,n}$. With the help of the multivariate Zeilberger algorithm we verify that the sequence d_n satisfies, for $n = 1, 2, \dots$,

$$(n+1)^3 d_{n+1} - 4(2n+1)(3n^2 + 3n + 1)d_n + 16n^3 d_{n-1} = 0.$$

The same recurrence is satisfied by [1, sequence (4.12) (ϵ)], so that comparing initial values proves that

$$d_n = \sum_{k=0}^n \binom{n}{k}^2 \binom{2k}{n}^2.$$

Since this makes positivity of the diagonal terms obvious, an affirmative answer to Question 1.1 when $d = 4$ would prove the conjectured positivity of $D(x, y, z, w)$.

Example 4.3 (Examples of Szegő and Koornwinder). Szegő proved, as a possible generalization of the function (10), the positivity of $1/e_3(1 - x, 1 - y, 1 - z, 1 - w)$; see [22, §3]. Upon rescaling, this is $h_{8/9, -16/27, 0}$. The positivity of the rational function $h_{8/9, -16/27, 0}$ can also be obtained, again via positivity preserving operators, see [21], from the positivity of Koornwinder's rational function [10, 14]

$$h_{0,4,-16}(x, y, z, w) = \frac{1}{1 - (x + y + z + w) + 4e_3(x, y, z, w) - 16xyzw}.$$

Using the multivariate Zeilberger algorithm, as in Example 4.2, we can show that the diagonal of $h_{0,4,-16}$ is given by the, obviously positive, sequence

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

This, again, is an Apéry-like sequence, namely [1, sequence (4.10) (β)].

Example 4.4. As shown in [12], the rational function

$$h_{0,0,c}(x, y, z, w) = \frac{1}{1 - (x + y + z + w) + cxyzw}$$

has non-negative coefficients if and only if $c \leq 24$. The condition $c \leq 24$ is necessary because the (diagonal) coefficient of $xyzw$ in $h_{0,0,c}$ is $24 - c$. On the other hand, asymptotic considerations, such as in Example 5.3 below, suggest that all but finitely many diagonal coefficients of $h_{0,0,c}$ are positive if $c < 27$.

This is the case $d = 4$ of a general conjecture from [10] mentioned in the introduction. In the general case, the rational function

$$\frac{1}{1 - (x_1 + x_2 + \dots + x_d) + cx_1 x_2 \cdots x_d}$$

can only be non-negative if $c \leq d!$ since the coefficient of $x_1 x_2 \cdots x_d$ is seen to be $d! - c$. It is conjectured in [10] that, for $d \geq 4$, the condition $c \leq d!$ is indeed sufficient, and it is claimed that the non-negativity follows from the non-negativity of the diagonal. On the other hand, some hypergeometric intuition suggests that the diagonal coefficients are eventually positive if $c < (d-1)^{d-1}$.

Example 4.5. In [12], the rational function

$$h_{0,64/27,0}(x, y, z, w) = \sum_{k,l,m,n \geq 0} a_{k,l,m,n} x^k y^l z^m w^n$$

is conjectured to be positive. As evidence, it is shown in [12], using cylindrical algebraic decomposition (CAD), that $a_{k,l,m,n} > 0$ whenever the sum of the smallest two indices is at most 12. On the other hand, we find that the diagonal coefficients satisfy a recurrence of order 3 and degree 6. While we could not discover any closed form expression for the diagonal terms, we have used CAD to prove that they are positive. Once more, an affirmative answer to Question 1.1 when $d = 4$ would therefore imply the conjectured positivity of $h_{0,64/27,0}$.

5. MULTIVARIATE ASYMPTOTICS

Multivariate asymptotics, as developed in [5, 16, 17, 19] and further illustrated in [18], is an approach to determine the asymptotics of the coefficients a_{n_1, \dots, n_d} of a multivariate generating function

$$h(x_1, \dots, x_d) = \sum_{n_1, \dots, n_d \geq 0} a_{n_1, \dots, n_d} x_1^{n_1} \cdots x_d^{n_d}$$

directly from h and its singular points.

In the sequel, we write $\mathbf{x} = (x_1, \dots, x_d)$. In the cases, we are presently interested in, $h = 1/p$ is the reciprocal of a polynomial $p(\mathbf{x})$. Denote with $\mathcal{V} \subseteq \mathbb{C}^d$ the *singular variety* defined by $p = 0$. A point $\mathbf{x} \in \mathcal{V}$ is smooth if $\nabla p(\mathbf{x}) = (\partial_1 p(\mathbf{x}), \dots, \partial_d p(\mathbf{x})) \neq \mathbf{0}$, where $\partial_j := \partial/\partial x_j$ for $j = 1, \dots, d$. The nonsmooth points can be comfortably computed using Gröbner bases, as detailed in [18, Section 4].

The next three examples indicate that rational functions which are on the boundary of positivity (that is, slightly perturbing one of its coefficients changes whether the function is positive) are intimately linked with rational functions that have nonsmooth points on their singular variety. This echoes the remark in [18] that, while for generic functions all points of the singular variety are smooth, “interesting applications tend not to be generic.”

Example 5.1. With $d = 2$, consider the case

$$h(x_1, x_2) = \frac{1}{1 - (x_1 + x_2) + ax_1 x_2}.$$

Then the singular variety has nonsmooth points if and only if $a = 1$. The nonsmooth point in the case $a = 1$ is $\mathbf{x} = (1, 1)$.

If $a < 1$ we may apply the machinery of [16] to find that

$$a_{n,n} \sim \frac{(1 + \sqrt{1-a})^{2n+1}}{2\sqrt{\pi n}\sqrt{1-a}}.$$

Example 5.2. With $d = 3$, consider the case

$$h(x_1, x_2, x_3) = \frac{1}{1 - (x_1 + x_2 + x_3) + a(x_1x_2 + x_2x_3 + x_3x_1) + bx_1x_2x_3}.$$

Then the singular variety has nonsmooth points if and only if

$$4a^3 - 3a^2 + 6ab + b^2 - 4b = 0.$$

Solving for b , this condition becomes $b = 2 - 3a \pm 2(1-a)^{3/2}$, which includes precisely the boundary in [21, Conjecture 1] explicitly describing the transition between positive rational functions and those with negative coefficients.

Example 5.3. With $d = 4$, consider the case

$$h(x_1, x_2, x_3, x_4) = \frac{1}{1 - e_1(\mathbf{x}) + ae_2(\mathbf{x}) + be_3(\mathbf{x}) + ce_4(\mathbf{x})}.$$

Then the singular variety has nonsmooth points if and only if

$$\begin{aligned} 0 = & (a^3 + 2ab - ac + b^2 + c)(64b^3 - 27(b^4 + c^2) + 6bc(2c - b) + c^3 \\ & - 54a(2b - c)(b^2 + c) + 18a^2(2b^2 + 10bc - c^2) - 54a^3(b^2 + c) + 81a^4c). \end{aligned}$$

We note that all the examples in Table 1, with the exception of $(0, 0, 24)$ which is not ‘natural’ as pointed out in Example 4.4, have nonsmooth points. The above factorization implies that, when

$$(17) \quad c = \frac{a^3 + 2ab + b^2}{a - 1},$$

the rational function h has nonsmooth points on its singular variety. The examples $(a, b, c) = (0, 4, -16)$ and $(8/9, -16/27, 0)$ from Table 1 are of this form.

Example 5.4. In the case $a = 0$ of (17), the rational function is

$$h_{0,b,-b^2} = \frac{1}{1 - (x + y + z + w) + b(yzw + xzw + xyw + xyz) - b^2xyzw}.$$

By direct computation, we observe that its Taylor coefficients $a_{r,s,t,u}$ are positive for all $0 \leq r, s, t, u \leq 20$ if and only if $b < 4.00796\dots$, which suggests that $h_{0,b,-b^2}$ is positive if and only if $b \leq 4$. Note that positivity was proven in [14] for the case $b = 4$. On the other hand, upon setting, say, $w = 0$, it follows from [21, Proposition 5] that positivity of $h_{0,b,-b^2}$ requires $b \leq 4$. However, it appears that the diagonal coefficients are positive for any $b \in \mathbb{R}$. Note that this sits nicely with and further illustrates Question 1.1. We note, however, that, for $b < 4$, the function $h_{0,b,-b^2}$ does not appear to be on the boundary of positivity.

Let a direction $\mathbf{n} = (n_1, \dots, n_d) \in \mathbb{Z}_{>0}^d$ be given. Among points on the singular variety \mathcal{V} , a special role is played by the *critical points* \mathbf{x} for \mathbf{n} , which are characterized [18, Proposition 3.11] by the d equations $p(\mathbf{x}) = 0$ and, for all $j = 1, \dots, d-1$,

$$(18) \quad n_d x_j \partial_j p(\mathbf{x}) = n_j x_d \partial_d p(\mathbf{x}).$$

We note the following consequence of [18, Theorem 3.16], which is a simple reformulation of [19, Proposition 5.1]; see the remark after [18, Theorem 3.16] for the uniqueness.

Proposition 5.5. *Let $\mathbf{n} \in \mathbb{Z}_{>0}^d$ be such that there is a smooth critical point for \mathbf{n} . If the rational function h is non-negative, then there is a unique critical point for \mathbf{n} in $\mathbb{R}_{>0}^d$.*

Example 5.6. For illustration, we use Proposition 5.5 to give an alternative proof of [21, Proposition 5], which states that the rational function

$$h(x, y, z) = \frac{1}{1 - (x + y + z) + bxyz}$$

is not non-negative if $b > 4$. Suppose that $b > 4$, in which case \mathcal{V} is smooth. A simple computation shows that h has three critical points for $\mathbf{n} = (1, 1, 1)$, namely, the points (c, c, c) , where c is a solution of

$$(19) \quad 1 - 3c + bc^3 = 0.$$

This cubic equation has discriminant $\Delta = 27b(4-b)$. The assumption $b > 4$ implies that $\Delta < 0$, which in turn implies that the equation (19) has only one real root. Since this real root is necessarily negative by the intermediate value theorem, we conclude that none of the three critical points for $(1, 1, 1)$ lies in $\mathbb{R}_{>0}^3$. By Proposition 5.5 it follows that h is not non-negative if $b > 4$.

Generalizing the approach taken in this example, we are able to show one part of [21, Conjecture 1].

Theorem 5.7. *For the rational function*

$$h(x, y, z) = \frac{1}{1 - (x + y + z) + a(xy + yz + zx) + bxyz}$$

to be non-negative it is necessary that $a \leq 1$ and $b \leq 2 - 3a + 2(1-a)^{3/2}$.

Proof. Upon setting $z = 0$, it follows from Section 2 that $a \leq 1$ is a necessary condition for h to be non-negative.

The defining equations (18) for critical points for $\mathbf{n} = (1, 1, 1)$ are equivalent to

$$(x - z)(ay - 1) = 0, \quad (y - z)(ax - 1) = 0.$$

There are therefore two kinds of critical points. Firstly, the points (c, c, c) , where c is a solution to

$$(20) \quad 1 - 3c + 3ac^2 + bc^3 = 0;$$

secondly, the points (x, y, z) where two coordinates equal $1/a$ and the third coordinate is $a(1-a)/(a^2+b)$.

We observe that the discriminant of the cubic equation (20) is negative if $a \leq 1$ and $b > 2 - 3a + 2(1-a)^{3/2}$. In that case, by the same argument as in the previous example, there are no critical points of the first kind in $\mathbb{R}_{>0}^3$. On the other hand, unless $b = -a^3$, there are three distinct critical points of the second kind, which either all lie in $\mathbb{R}_{>0}^3$ or all lie outside $\mathbb{R}_{>0}^3$.

Suppose that $a \leq 1$ and $b > 2 - 3a + 2(1-a)^{3/2}$. Then the case $b = -a^3$ occurs only if $a < -3$, in which case the critical points of the second kind lie outside $\mathbb{R}_{>0}^3$. We conclude that h cannot have a unique critical point in $\mathbb{R}_{>0}^3$. Since, by Example 5.2, all points on the singular variety of h are smooth, the claim therefore follows from Proposition 5.5. \square

Note the special role played by the diagonal direction $\mathbf{n} = (1, 1, 1)$, though the present proof does use global information when applying Proposition 5.5.

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REFERENCES

- [1] G. ALMKVIST, D. VAN STRATEN and W. ZUDILIN, Generalizations of Clausen's formula and algebraic transformations of Calabi–Yau differential equations, *Proc. Edinburgh Math. Soc.* **54** (2011), 273–295.
- [2] R. ASKEY, Certain rational functions whose power series have positive coefficients. II, *SIAM J. Math. Anal.* **5** (1974), 53–57.
- [3] R. ASKEY and G. GASPER, Certain rational functions whose power series have positive coefficients, *Amer. Math. Monthly* **79** (1972), 327–341.
- [4] R. ASKEY and G. GASPER, Convolution structures for Laguerre polynomials, *J. Analyse Math.* **31** (1977), 48–68.
- [5] Y. BARYSHNIKOV and R. PEMANTLE, Asymptotics of multivariate sequences, part III: Quadratic points, *Adv. Math.* **228** (2011), 3127–3206.
- [6] B. C. BERNDT, *Ramanujan's Notebooks, Part V* (Springer-Verlag, New York, 1998).
- [7] J. M. BORWEIN and P. B. BORWEIN, A cubic counterpart of Jacobi's identity and the AGM, *Trans. Amer. Math. Soc.* **323** (1991), 691–701.
- [8] S. B. EKHAD, A linear recurrence equation for the diagonal coefficients of the power series of $1/(1-x-y-z+4xyz)$, *Preprint* (2012), 1 p.; available from <http://www.math.rutgers.edu/~zeilberg/tokhniot/oMultiAlmkvistZeilberger3>.
- [9] J. FRANEL, On a question of Laisant, *L'Intermédiaire des Mathématiciens* **1** (1894), 45–47.
- [10] J. GILLIS, B. REZNICK and D. ZEILBERGER, On elementary methods in positivity theory, *SIAM J. Math. Anal.* **14** (1983), 396–398.
- [11] M. E. H. ISMAIL and M. V. TAMHANKAR, A combinatorial approach to some positivity problems, *SIAM J. Math. Anal.* **10** (1979), 478–485.
- [12] M. KAUSERS, Computer algebra and power series with positive coefficients, in: *Formal Power Series and Algebraic Combinatorics 2007* (Nankai University, Tianjin, China, 2007), 7 pp.; available from <http://igm.univ-mlv.fr/~fpsac/FPSAC07/SITE07/PDF-Proceedings/Talks/20.pdf>.
- [13] M. KAUSERS and D. ZEILBERGER, Experiments with a positivity-preserving operator, *Experiment. Math.* **17** (2008), 341–345.

- [14] T. KOORNWINDER, Positivity proofs for linearization and connection coefficients of orthogonal polynomials satisfying an addition formula, *J. London Math. Soc.* (2) **18** (1978), 101–114.
- [15] R. S. MAIER, Algebraic hypergeometric transformations of modular origin, *Trans. Amer. Math. Soc.* **359** (2007), 3859–3885.
- [16] R. PEMANTLE and M. C. WILSON, Asymptotics of multivariate sequences. I. Smooth points of the singular variety, *J. Combin. Theory Ser. A* **97** (2002), 129–161.
- [17] R. PEMANTLE and M. C. WILSON, Asymptotics of multivariate sequences. II. Multiple points of the singular variety, *Combin. Probab. Comput.* **13** (2004), 735–761.
- [18] R. PEMANTLE and M. C. WILSON, Twenty combinatorial examples of asymptotics derived from multivariate generating functions, *SIAM Rev.* **50** (2008), 199–272.
- [19] A. RAICHEV and M. C. WILSON, Asymptotics of coefficients of multivariate generating functions: improvements for smooth points, *Electron. J. Combin.* **15** (2008), R89, 17 pp.
- [20] A. D. SCOTT and A. D. SOKAL, Complete monotonicity for inverse powers of some combinatorially defined polynomials, *Preprint arXiv: 1301.2449 [math.CO]* (2013), 79 pp.
- [21] A. STRAUB, Positivity of Szegő’s rational function, *Adv. Appl. Math.* **41** (2008), 255–264.
- [22] G. SZEGÖ, Über gewisse Potenzreihen mit lauter positiven Koeffizienten, *Math. Z.* **37** (1933), 674–688.

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