Approximating Mills ratio

ARMENGOL GASULL AND FREDERIC UTZET

Departament de Matemàtiques, Edifici C, Universitat Autònoma de Barcelona, 08193 Bellaterra (Barcelona) Spain. E-mails: gasull@mat.uab.cat, utzet@mat.uab.cat

Abstract.
Consider the Mills ratio $f(x) = \big(1 - \Phi(x)\big)/\phi(x)$, $x \geq 0$, where ϕ is the density function of the standard Gaussian law and Φ its cumulative distribution. We introduce a general procedure to approximate f on the whole $[0, \infty)$ which allows to prove interesting properties where f is involved. As applications we present a new proof that $1/f$ is strictly convex, and we give new sharp bounds of f involving rational functions, functions with square roots or exponential terms. Also Chernoff type bounds for the Gaussian Q–function are studied.

Keywords: Gaussian law, Mills ratio, error function, Gaussian Q–function

1 Introduction

Recall that the Mills ratio (Mills [22]) is the function

$$f(x) = \frac{1 - \Phi(x)}{\phi(x)} = e^{\frac{x^2}{2}} \int_x^\infty e^{-\frac{t^2}{2}}\, dt,\ x \geq 0, \tag{1}$$

where $\phi(x) = e^{-x^2/2}/\sqrt{2\pi}$ is the density function of a standard Gaussian law and $\Phi(x) = \int_{-\infty}^x \phi(t)\, dt$ its cumulative distribution function. The study of this function is much older than Mills [22], and through its relation with the function

$$F(x) = e^{x^2} \int_x^\infty e^{-t^2}\, dt \tag{2}$$

given by

$$f(x) = \sqrt{2}\, F(x/\sqrt{2}),$$

its introduction can be traced back to Laplace (1805) [21, Livre X, Chap. 1, n$^{\text{o}}$ 5], while he was analyzing different hypotheses related with the refraction of the light in the atmosphere. As we will comment later, Laplace gave many of the essential results, like the continued fraction and the asymptotic expansion. Moreover, since the function F is related with the error function, and also with the upper incomplete Gamma function of parameter $1/2$, properties of Mills ratio are spread between papers and books of Probability and Statistics, Mathematical Analysis, Numerical Analysis, etc, and many results have been discovered and rediscovered by different authors.

In the first part of this paper we collect, in a short, unified and self-contained way, some known results about the approximation of f by rational funcions. In particular, we prove the surprising fact that the convergents of the continued fraction of f give, at the same time, the expression of its n^{th}-derivative.

In a second part, joining the rational bounds for $f(x)$ when x is large, with a Taylor formula for small x, we construct effective bounds for f on the whole $[0, \infty)$. From that, we introduce a general procedure to prove properties where f is involved; this procedure consists on the reduction to the problem at hand to the control of the real roots of a polynomial with rational coefficients, which can be done using rigorous analytic methods based on the Sturm Theorem (see the Appendix for more details on that theorem).

As a first application we prove that the reciprocal function of Mills ratio $1/f$ is strictly convex. This result was implicitly conjectured by Birnbaum [5] in 1950 (see Subsection 3.2) and demonstrated few years later independently by Sampford [29] and Shenton [31]. We stress that, in contrast with known proofs, we apply a general procedure which, as we will see, can be useful in many other problems.

As a second application we study lower and upper bounds for f of the form

$$\psi_{a,b,c}(x) = \frac{a}{\sqrt{x^2 + b} + cx}.$$

These functions have the same type of asymptotic expansion as f when $x \to \infty$, and then very sharp bounds for f can be obtained. These bounds are important because they give very good estimations of the Gaussian cumulative probability distribution. We review in a systematic way known bounds of this type, and construct other new.

Finally, we shortly present new families of simple bounds of f of the form $a/(b+x)$, $(a+bx)/(c+dx+x^2)$ and $\big(1-\exp(-ax)\big)/bx$. We also comment on Chernoff type bounds $a\exp(-bx^2)$ for the function $\int_x^\infty \exp(-t^2/2)\,dt/\sqrt{2\pi}$, called the Gaussian Q–function in engineering literature. All these properties can be proved by using our methodology.

2 Approximation of Mills ratio by rational functions

2.1 Notations and main results

Starting from $f'(x) = xf(x) - 1$, it follows that the n^{th}-derivative of f, $n \geq 1$, satisfies

$$f^{(n)}(x) = P_n(x)f(x) - Q_n(x), \tag{3}$$

for some polynomials P_n and Q_n, with non negative integer coefficients and respective degrees n and $n-1$. We prove:

Theorem 1. *Let P_n and Q_n be the polynomials defined by* (3) *where f is the Mills ratio* (1)*. Then, for all $n \geq 1$ and $x \geq 0$,*

$$0 < (-1)^n \frac{f^{(n)}(x)}{P_n(x)} = (-1)^n \left(f(x) - \frac{Q_n(x)}{P_n(x)} \right) < \frac{n!}{x^{2n+1}}. \tag{4}$$

Moreover, for all $x > 0$, when $m \to \infty$,

$$\frac{Q_{2m}(x)}{P_{2m}(x)} \nearrow f(x) \quad \text{and} \quad \frac{Q_{2m+1}(x)}{P_{2m+1}(x)} \searrow f(x).$$

Our proof is similar to the approach presented in the unpublished (as far as we know) work of Kouba ([18]) that we discovered after preparing a first version of this paper.

As a corollary of Theorem 1 we obtain:

Corollary 2.

(i) The Mills ratio f is completely monotone.

(ii) The rational functions Q_n/P_n are the convergents of the continued fraction expansion of f.

(iii) The rational functions Q_n/P_n are the Padé–Laurent approximants of f at infinity.

(iv) The polynomial $P_n(x)$ coincides with $He_n(ix)/i^n$, where $i^2 = -1$, and $He_n(x)$ is the monic Hermite polynomial of order n with respect to the weight function $e^{-x^2/2}$.

Item *(i)* is already known, see the comments below. The convergents and the Padé–Laurent approximants of f are also known, but they are obtained using a different method. We obtain them simply using equality (3). Let us comment with more detail all the items of the corollary.

Recall that a function $h : (0,\infty) \to \mathbb{R}$ is called *completely monotone* if it is of class $\mathcal{C}^\infty$ and for all $n \geq 0$,

$$(-1)^n h^{(n)}(x) \geq 0, \; x > 0,$$

where $h^{(0)} = h$. Completely monotone functions and the related Bernstein functions constitute a topic of permanent interest due to its apparition in several different areas of Mathematics and its many applications; for a complete treatise see Schilling *et al.* [30].

The result stated in item *(i)* was proved by Baricz [3]. Its proof is based on the following nice equality

$$f(x) = e^{\frac{x^2}{2}} \int_x^\infty e^{-\frac{t^2}{2}}\, dt = \int_0^\infty e^{-xt} e^{-\frac{t^2}{2}}\, dt, \tag{5}$$

that already appears in Ray and Pitman [27, Formula (9)]. From this equality the sign of the n^{th} derivative is simply obtained using the right-hand side expression of f. Recall that Bernstein Theorem (see Schilling *et al.* [30, Theorem 1.4]) characterizes completely monotone functions as the ones that are the Laplace transform of a (univocally determinate) measure on $[0, \infty)$. Equality (5) gives explicitly this measure.

In item *(ii)* we prove that Q_n/P_n are the convergents of the continued fraction expansion of f:

$$f(x) = \cfrac{1}{x + \cfrac{1}{x + \cfrac{2}{x + \cfrac{3}{x + \cdots}}}}. \tag{6}$$

The expansion corresponding to the function F given in (2) was obtained by Laplace [21, Livre X, Chap. 1, n$^{\text{o}}$ 5] and the continued fraction (6) can be easily deduced from Laplace's one. For a direct proof of (6) see Small [32, Section 3.5].

One of the main steps in the proof of Theorem 1 and of item *(ii)* is to show that $\{P_n(x)\}_n$ and $\{Q_n(x)\}_n$ satisfy some second order recurrences, see Lemma 3. We obtain these recurrences by using that the differential equation $y'(x) - xy(x) = 1$ has no rational solutions. It is interesting to comment that this is one of the key points in the celebrated Liouville's proof that the distribution function of the Gaussian law has no primitive which can be expressed in terms of elementary functions, see Remark 4.

In item *(iii)* we show that the rational functions Q_n/P_n are some Padé–Laurent approximants of f at infinity. Similar results appear in [25]. In fact the asymptotic expansion of f at infinity is (see Small [32, p. 44])

$$f(x) \sim \frac{1}{x} - \frac{1}{x^3} + \frac{1\cdot 3}{x^5} - \frac{1\cdot 3\cdot 5}{x^7} + \cdots,\ x \to \infty. \tag{7}$$

This expansion also comes from Laplace [21, Livre X, Chap. 1, n$^{\text{o}}$ 5] (with the same comments as above with respect to the function involved). The bounds for f deduced from (7) are widely used in Probability and Statistics; for example, Hall [14] uses the first two terms as a key ingredient to get the rate of convergence in the supremum metric of the maxima of standard normal random variables to Gumbel law. Denote by $J_n(x)$ the finite expansion of $f(x)$ up to $1/x^{2n-1}$ deduced from (7): $J_1(x) = 1/x$, and

$$J_n(x) = \frac{1}{x} - \frac{1}{x^3} + \cdots + (-1)^{n+1}\frac{(2n-3)!!}{x^{2n-1}}, \quad \text{for } n \geq 2, \tag{8}$$

It is well known (see Small [32, Section 2.3]) that the error term of the finite expansion is bounded by the first neglected term, that is,

$$0 < (-1)^n \left(f(x) - J_n(x)\right) < \frac{(2n-1)!!}{x^{2n+1}}. \tag{9}$$

Since $n! < (2n-1)!!$, the functions $Q_n(x)/P_n(x)$ seem to approach faster f than the functions $J_n(x)$ (see Theorem 1). This turns out to be true, see Lemma 5. A possible explanation of this fact comes from item *(iii)* of Corollary 2. As often happens the Padé approximants give better approximation of the function than truncating the corresponding Taylor series.

We thank Iain Johnstone for pointing out the property given in item *(iv)*. It was missed in a first version of this work. From the explicit expression of the Hermite polynomials NIST [24, Formulas 18.5.13 and 18.7.12] it is deduced that

$$P_n(x) = n! \sum_{k=0}^{[n/2]} \frac{x^{n-2k}}{2^k k!(n-2k)!}. \tag{10}$$

Property *(iv)* and expression (10) appear in Kouba [18], where also an explicit expression of Q_n is given.

2.2 Proof of Theorem 1 and Corollary 2

We first compile several properties of the polynomials introduced in (3), see also Kouba [18].

Lemma 3. *Let P_n and Q_n be the polynomials defined by* (3)*.*

(a) It holds that

$$P_n(x) = xP_{n-1}(x) + (n-1)P_{n-2}(x),\ n \geq 2, \tag{11}$$

with initial conditions $P_0(x) = 1$ and $P_1(x) = x$, and

$$Q_n(x) = xQ_{n-1}(x) + (n-1)Q_{n-2}(x),\ n \geq 2, \tag{12}$$

with initial conditions $Q_0(x) = 0$ and $Q_1(x) = 1$. In particular, both polynomials P_n and Q_n are monic and their coefficients are nonnegative integers.

(b) For $n \geq 1$,

$$P_n'(x) = nP_{n-1}(x) \qquad \text{and} \qquad Q_n'(x) = xQ_n(x) + nQ_{n-1}(x) - P_n(x). \tag{13}$$

(c) For $n \geq 1$,

$$Q_n(x)P_{n-1}(x) - Q_{n-1}(x)P_n(x) = (-1)^{n+1}(n-1)!. \tag{14}$$

Proof. (a) From (1) and the equalities $\Phi'(x) = \phi(x)$ and $\phi'(x) = -x\phi(x)$, we arrive to

$$f'(x) = xf(x) - 1 \qquad \text{and} \qquad f''(x) = (x^2+1)f(x) - x. \tag{15}$$

In general, for $n \geq 2$, thanks to Leibnitz formula for the derivative of order n of a product of functions, we have the recurrence

$$f^{(n)}(x) = xf^{(n-1)}(x) + (n-1)f^{(n-2)}(x), \tag{16}$$

where $f^{(0)} = f$. Given the form of f' and f'' in (15), it is deduced by induction that (3) holds, where P_n and Q_n are polynomials of degree n and $n-1$ respectively (for $n \geq 1$). For $n = 0$ the corresponding polynomials are $P_0(x) = 1$ and $Q_0(x) = 0$. The first polynomials are

$$P_1(x) = x,\ P_2(x) = x^2+1,\ P_3(x) = x^3+3x,\ P_4(x) = x^4+6x^2+3,\ P_5(x) = x^5+10x^3+15x,$$

and

$$Q_1(x) = 1,\ Q_2(x) = x,\ Q_3(x) = x^2+2,\ Q_4(x) = x^3+5x,\ Q_5(x) = x^4+9x^2+8.$$

Note that from (3) and (16),

$$\big(P_n(x) - xP_{n-1}(x) - (n-1)P_{n-2}(x)\big)f(x) = Q_n(x) - xQ_{n-1}(x) - (n-1)Q_{n-2}(x). \tag{17}$$

For any n given, the factor $P_n(x) - xP_{n-1}(x) - (n-1)P_{n-2}(x)$ is a polynomial of degree n, and thus, if it is not identically zero we get that f is a rational function. On the other hand remember that by (15), $f'(x) = xf(x) - 1$. It is not difficult to prove that this equation has no rational solutions: f cannot be a polynomial by degree considerations. Hence f should have a (real or complex) pole. This pole is also present in f' but with a different order, giving again the impossibility of f to be a solution of the equation. Then, the polynomials P_n and Q_n follow the recurrences (11) and (12) as we wanted to prove.

(b) Notice that

$$\begin{aligned} P_{n+1}(x)f(x) - Q_{n+1}(x) &= f^{(n+1)}(x) = \big(P_n(x)f(x) - Q_n(x)\big)' \\ &= P_n'(x)f(x) + P_n(x)f'(x) - Q_n'(x) \\ &= \big(P_n'(x) + xP_n(x)\big)f(x) - \big(P_n(x) + Q_n'(x)\big). \end{aligned}$$

Then,

$$P_{n+1}(x) = P_n'(x) + xP_n(x) \qquad \text{and} \qquad Q_{n+1}(x) = P_n(x) + Q_n'(x). \tag{18}$$

Joining the above left equality with the recurrence (11) for P_{n+1} it follows the first formula in (13). Similarly, combining the right one with the recurrence for Q_{n+1} in (12), gives the second equality in (13).

(c) Equality (14) follows easily by induction, changing P_n and Q_n by their corresponding expressions given in (11) and (12), respectively. □

Remark 4. Our proof of item (a) uses one of the steps of the proof that $\int e^{-x^2/2}\,dx$ has no primitive expressible in terms of elementary functions. To realize this fact it is convenient a short comment on this proof. It goes back to the work of Liouville 1835 ([19]) and is a consequence of a much more general result. Liouville Theorem together with its proof can also be consulted for instance in Rosenlicht [28]. In Conrad [9], there is a simple and nice corollary of Liouville's result: *Consider a function $F(x) = p(x)e^{q(x)}$, where both p and q are rational functions with p not identically zero and q not constant. Then F can be integrated in elementary terms if and only if there exists a rational function R such that*

$$R'(x) + q'(x)R(x) = p(x). \tag{19}$$

Moreover, in this case $\int p(x)e^{q(x)}dx = R(x)e^{q(x)} + k$ for some constant k. Notice that for the integral $\int e^{-x^2/2}\,dx$, the differential equation (19) is precisely the differential equation (15) satisfied by f, which, as we have already argued in the proof of the above lemma, has no rational solutions.

Proof of Theorem 1. We start proving the inequality

$$(-1)^n \frac{f^{(n)}(x)}{P_n(x)} = (-1)^n \left(f(x) - \frac{Q_n(x)}{P_n(x)} \right) > 0. \tag{20}$$

When n is even we have to see that (for n odd, reverse the inequality), $f(x) > Q_n(x)/P_n(x)$, or equivalently,

$$1 - \Phi(x) > \phi(x)\frac{Q_n(x)}{P_n(x)}. \tag{21}$$

This inequality is proved with the clever argument that Feller ([13, page 175]) uses to deduce the asymptotic expansion (7): We will see that the negative of the derivatives of those of (21) satisfy the inequality

$$\phi(x) > -\left(\phi(x)\frac{Q_n(x)}{P_n(x)} \right)' \tag{22}$$

(reversed inequality if n is odd). Hence, integrating both members of that inequality from x to infinity we obtain (21).

To prove (22) we first claim that for every $n \geq 1$,

$$xP_n(x)Q_n(x) - Q_n'(x)P_n(x) + Q_n(x)P_n'(x) = P_n^2(x) + (-1)^{n+1}n!. \tag{23}$$

Using this claim we get that the right hand side of (22) is

$$\begin{aligned} x\phi(x)\frac{Q_n(x)}{P_n(x)} - \phi(x)\frac{Q_n'(x)P_n(x) - Q_n(x)P_n'(x)}{P_n^2(x)} \\ = \phi(x)\left(\frac{xP_n(x)Q_n(x) - Q_n'(x)P_n(x) + Q_n(x)P_n'(x)}{P_n^2(x)} \right) = \phi(x)\left(1 + \frac{(-1)^{n+1}n!}{P_n^2(x)} \right). \end{aligned}$$

Then, (22) for n even, and the reversed inequality for n odd, will follow.

To prove the claim, in (23), we change P_n' and Q_n' by their corresponding expressions in (13). It turns out that to prove (23) is equivalent to prove (14). Hence, from (c) in Lemma 3, the proof of (20) is complete.

Let us prove the right-hand inequality of (4). For n even, thanks to identity (14),

$$\frac{Q_{n+1}(x)}{P_{n+1}(x)} - \frac{Q_n(x)}{P_n(x)} = \frac{n!}{P_{n+1}(x)P_n(x)}. \tag{24}$$

Recall that the polynomials P_n are monic and all their coefficients are nonnegative. Then $P_{n+1}(x)P_n(x) > x^{2n+1}$. Thus,

$$0 < \frac{Q_{n+1}(x)}{P_{n+1}(x)} - \frac{Q_n(x)}{P_n(x)} < \frac{n!}{x^{2n+1}},$$

and the result follows because

$$\frac{Q_{2n}(x)}{P_{2n}(x)} < f(x) < \frac{Q_{2n+1}(x)}{P_{2n+1}(x)}. \tag{25}$$

Finally, to prove that when $x > 0$,

$$\lim_{n\to\infty} \frac{P_n(x)}{Q_n(x)} = f(x),$$

we will need a suitable lower bound for $P_{n+1}(x)P_n(x)$. We will consider the independent term and the coefficient of x of $P_n(x)$. By (10), $P_n(0) = (n-1)!!$, if n is even, and 0 otherwise, where $k!!$ is the double factorial of a positive integer, defined recurrently for $k \geq 2$ as $k!! = k \times (k-2)!!$, with the conventions $0!! = 1!! = 1$. Also, $P_n[1] = n!!$ if n is odd, and 0 otherwise.

Using again that all coefficient of P_n are non negative, and $P_{n+1}(0) = 0$, for every $x > 0$, we can bound the product $P_{n+1}(x)P_n(x)$ in the following way:

$$P_{n+1}(x)P_n(x) > xP_{n+1}[1]P_n(0) = x\,(n+1)!!(n-1)!!.$$

Thus, for n even, equality (24) gives

$$0 < \frac{Q_{n+1}(x)}{P_{n+1}(x)} - \frac{Q_n(x)}{P_n(x)} < \frac{n!}{x(n+1)!!(n-1)!!}.$$

Fixed n, the right hand side goes to 0 when $x \to \infty$, and fixed $x > 0$, by Stirling formula, it goes to 0 when $n \to \infty$. For any $x > 0$, the monotonicity of the even and odd terms of the sequence $Q_n(x)/P_n(x)$ is an straightforward consequence of item (c) of Lemma 3. Then the theorem follows. □

Proof of Corollary 2. (i) Notice that because $P_n(x) > 0$ for all $x > 0$ the fact that $(-1)^n f^{(n)}(x) > 0$ for all $x > 0$ is a straightforward consequence of (4).

(ii) Consider the continued fraction (6) of f. The *three terms recurrence relation* that follow the n^{th} numerator and the n^{th} denominator of a continued fraction (see Cuyt *et al.* [11, page 13]) are exactly the recurrences for P_n and Q_n given by (11) and (12). So Q_n/P_n is the n convergent of (6). Then, the properties of continued fractions can be used to give an alternative proof of items (b) and (c) of Lemma 3; see Pinelis [25] and Shenton [31]. In fact, there is a natural procedure for finding a continued fraction expansion for a function satisfying a first order differential equation with polynomials entries that goes back to Laguerre, see [20]. Notice that our Mills ratio f belongs to this class of functions.

(iii) Given a generic function S we define $\widetilde{S}(y) = S(1/y)$. Then, from (7), (8) and (9) it holds that

$$\widetilde{f}(y) = \widetilde{J}_n(y) + O(y^{2n+1}), \tag{26}$$

where $\widetilde{J}_n(y) = y - y^3 + \cdots + (-1)^{n+1}(2n-3)!!y^{2n-1}$, and, as usual, we write that $k(x) = O(h(x))$ when $x \to \infty$ if there is a point x_0 and a constant C such that $|k(x)| \leq Ch(x)$, for all $x > x_0$. Consider now the rational functions

$$\frac{\widetilde{Q}_{2m}(y)}{\widetilde{P}_{2m}(y)} = y\,\frac{R_{m-1}(y^2)}{S_m(y^2)}, \qquad \frac{\widetilde{Q}_{2m+1}(y)}{\widetilde{P}_{2m+1}(y)} = y\,\frac{T_m(y^2)}{U_m(y^2)},$$

where R_j, S_j, T_j and U_j are polynomials of degree j. Notice that by Theorem 1, $\widetilde{Q}_n(y)/\widetilde{P}_n(y) - \widetilde{f}(y) = O(y^{2n+1})$. Hence, by (26),

$$\widetilde{J}_n(y) - \frac{\widetilde{Q}_n(y)}{\widetilde{P}_n(y)} = O(y^{2n+1}).$$

This equality implies that $\widetilde{Q}_n(y)/\widetilde{P}_n(y)$ are the Padé approximants of $\widetilde{J}_n(y)$ and $\widetilde{f}(y)$ at the origin, of order $[n-1,n]$ when n is even and of order $[n,n-1]$ when n is odd because all the derivatives until order $2n$ at the origin coincide. Hence the corresponding $Q_n(x)/P_n(x)$ are the Padé–Laurent approximants of $f(x)$ at infinity. Finally, notice that by symmetry arguments, when n is even the Padé approximants of orders $[n-1,n], [n-1,n+1], [n,n]$ and $[n,n+1]$ coincide. Similarly, when n is odd the approximants that conicide are the ones having orders $[n,n-1], [n,n]$ and $[n+1,n]$.

(iv) The recurrence of the monic Hermite polynomials with respect to the weight function $e^{-x^2/2}$ is (see NIST [24, Table 18.9(ii)])

$$He_n(x) = xHe_{n-1}(x) - (n-1)He_{n-2}(x),$$

with initial conditions $He_0(x) = 1$ and $He_1(x) = x$. Comparing with the recurrence of P_n given in (11) the property is easily proved. $\square$

2.3 A comparison between J_n and Q_n/P_n

Notice that by (8),

$$J_{n+1}(x) = J_n(x) + (-1)^{n+2}\frac{(2n-1)!!}{x^{2n+1}} \quad \text{and} \quad J_n'(x) = xJ_{n+1}(x) - 1. \tag{27}$$

Next result shows that J_n approximates worst f that Q_n/P_n. This fact corroborates once more the general believe that Padé approximants are better than the corresponding truncated series.

Lemma 5. *For $x > 0$ and $m \geq 1$,*

$$J_{2m}(x) < \frac{Q_{2m}(x)}{P_{2m}(x)} < f(x) < \frac{Q_{2m+1}(x)}{P_{2m+1}(x)} < J_{2m+1}(x).$$

Proof. As in the proof of Theorem 1, we use again the idea from Feller ([13, page 175]): We prove that for n even (the proof for n odd is analogous),

$$\phi(x)J_n(x) < \phi(x)\frac{Q_n(x)}{P_n(x)}.$$

To this end, it suffices to check the inequality with the negatives of the derivatives of both sides of previous inequality,

$$-\phi(x)J_n'(x) + x\phi(x)J_n(x) < -\phi(x)\left(\frac{Q_n(x)}{P_n(x)}\right)' + x\phi(x)\frac{Q_n(x)}{P_n(x)}, \tag{28}$$

and then integrate from x to infinite. By (27) the left hand side of (28) is

$$-\phi(x)J_n'(x) + x\phi(x)J_n(x) = \phi(x)\left(1 + x\big(J_n(x) - J_{n+1}(x)\big)\right) = \phi(x)\left(1 - \frac{(2n-1)!!}{x^{2n}}\right).$$

Therefore, from the above equality and (23), the inequality (28) is equivalent to

$$\frac{n!}{P_n^2(x)} < \frac{(2n-1)!!}{x^{2n}},$$

which is evident. $\square$

Remark 6. Note that J_{2n} is negative in an interval $[0,\alpha_n)$ for an increasing sequence of positive numbers $\{\alpha_n\}_n$; on the contrary, $Q_n(x)/P_n(x) > 0$ for $x > 0$, see Figure 1. This is important when we want to bound expressions involving f; see the proof of Theorem 9.

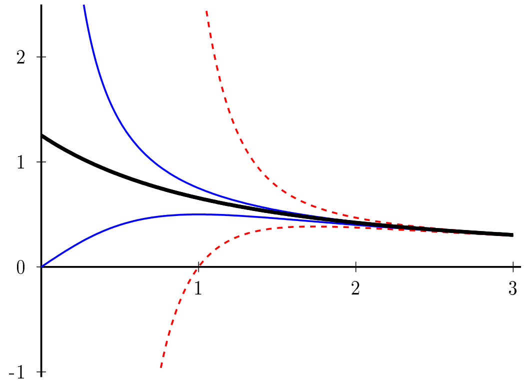

Figure 1. Bold solid line: function f. Upper and lower light solid lines: rational functions Q_3/P_3 and Q_2/P_2, respectively. Upper and lower dashed lines: rational functions J_3 and J_2 respectively.

3 An approximation procedure

3.1 Taylor formula

To approach f in a neighborhood of the origin we need to compute its Taylor expansion at $x = 0$. The alternating of signs of the derivatives $f^{(n)}$ implies that the Taylor series of f at zero enjoys very nice properties. Let T_n be the Taylor polynomial of f of order n at zero. Using the Lagrange remainder, for all $x \geq 0$

$$f(x) = T_n(x) + \frac{1}{(n+1)!}\, f^{(n+1)}(x_0)\, x^{n+1},$$

for some $x_0 \in [0, x]$. Then, thanks to the sign of $f^{(n+1)}(x_0)$ given in Theorem 1, if n is odd, for $x > 0$, $T_n(x) < f(x) < T_{n+1}(x)$. What is more, given that if n is odd, $f^{(n)}$ is increasing and $f^{(n+1)}$ is decreasing, and if n is even happens the contrary, the remainder of T_n and T_{n+1} can be expressed in a more convenient form, and

$$f(x) = T_n(x) + \xi_n \frac{1}{(n+1)!}\, f^{(n+1)}(0)\, x^{n+1},$$

where $\xi_n \in (0, 1)$. Then it is said that the Taylor series is *enveloping* (see Small [32, Section 2.3]).

The coefficients of the Taylor series are computed from $f^{(n)}(0) = P_n(0)f(0) + Q_n(0)$ and are

$$f^{(n)}(0) = \begin{cases} -(n-1)!!, & \text{if } n \text{ is odd,} \\ (n-1)!!\,\dfrac{\sqrt{2\pi}}{2}, & \text{if } n \text{ is even.} \end{cases}$$

Notice that these values of $f^{(n)}(0)$ can also be obtained from equality (5). We summarize the above results in the following lemma:

Lemma 7. *The Taylor series of f at 0 is convergent in the whole $[0, \infty)$ and it is given by*

$$f(x) = \frac{\sqrt{2\pi}}{2} - x + \frac{\sqrt{2\pi}}{4}\, x^2 - \frac{1}{3}\, x^3 + \frac{\sqrt{2\pi}}{16}\, x^4 - \frac{1}{15}\, x^5 + \cdots,$$

where the coefficient of x^n is

$$\begin{cases} \dfrac{\sqrt{2\pi}}{2\, n!!}, & \textit{if } n \textit{ is even,} \\ \\ -\dfrac{1}{n!!}, & \textit{if } n \textit{ is odd,} \end{cases}$$

and it is enveloping. In particular, for all $n \geq 1$ and for every $x > 0$, $T_{2n-1}(x) < f(x) < T_{2n}(x)$ and the remainder of the Taylor polynomial is bounded in absolute value by the first neglected term.

Combining this lemma and Theorem 1 we get the following proposition:

Proposition 8. *For any positive integer numbers k, ℓ, m, n and $x > 0$ it holds that*

$$\max\left(T_{2k-1}(x), \frac{Q_{2\ell}(x)}{P_{2\ell}(x)}\right) < f(x) < \min\left(T_{2m}(x), \frac{Q_{2n-1}(x)}{P_{2n-1}(x)}\right).$$

3.2 The approximation procedure in action: $1/f$ is strictly convex

As a first application we present a new proof of the following theorem:

Theorem 9. *The reciprocal function of Mills ratio $1/f$ is strictly convex.*

As we will see, the proof will be reduced to show that the function $g(x) := 2 + x^2 f^2(x) - f^2(x) - 3xf(x)$ is strictly positive for all $x > 0$. To prove this, we will search for suitable piecewise rational functions, $\underline{R}$ and $\overline{R}$, with coefficients in $\mathbb{Q}^+ \cup \{0\}$ and well defined on $[0, \infty)$, such that for all $x > 0$ it holds that

$$0 < \underline{R}(x) < f(x) < \overline{R}(x).$$

Define $\widehat{g}(x) := 2 + x^2\, \underline{R}^2(x) - \overline{R}^{\,2}(x) - 3x\overline{R}\,(x)$. Then $g(x) > \widehat{g}(x)$ and proving that for $x > 0$, $\widehat{g}(x) > 0$, the result will follow.

The fact that all the coefficients are rational is crucial in our approach because the numerator of $\widehat{g}$ will be a polynomial with rational coefficients and then rigorous analytic methods, like Sturm Theorem, can be used to prove the inequality. We recall Sturm Theorem in the Appendix.

These piecewise functions will be constructed from the class of functions appearing in the statement of Proposition 8. More concretely, to get $\underline{R}$ and $\overline{R}$ we will use modified Taylor polynomials in $[0, 1]$ and the fractions Q_n/P_n given in the remainder unbounded interval.

Proof of Theorem 9. We have that

$$\left(\frac{1}{f(x)}\right)'' = \frac{2 + x^2 f^2(x) - f^2(x) - 3xf(x)}{f^3(x)} = \frac{g(x)}{f^3(x)}.$$

It suffices to prove that $g(x) > 0$ (this was Birnbaum conjecture [5]). As we have already explained, we will bound below g by a strictly positive function in two steps: for $x \in [0, 1]$ using Taylor formulas, and for $x > 1$ using adequate rational functions Q_n/P_n.

Step 1. $x \in [0, 1]$**.** By Proposition 8, $T_7(x) < f(x) < T_8(x)$. Since the polynomials T_n involve the irrational number $\sqrt{2\pi}$ in the positive coefficients, we look for convenient rational approximations, which are

$$\frac{5}{2} < \sqrt{2\pi} < \frac{188}{75}. \tag{29}$$

Such fractions are obtained computing the continued fraction of $\sqrt{2\pi}$, $[2, 1, 1, 37, 4, 1, 1 \ldots]$ and the corresponding convergents $2, 3, 5/2, 188/75, 757/302, \ldots$

Denote by $T_{7,\ell}(x)$ (respectively, $T_{8,u}(x)$) the polynomial $T_7(x)$ (resp. $T_8(x)$) with the fraction in the left hand side of (29) (respectively in the right hand side) instead of the number $\sqrt{2\pi}$. We have that for $x \in [0, 1]$,

$$0 < T_{7,\ell}(x) < T_7(x) < f(x) < T_8(x) < T_{8,u}(x),$$

where

$$T_{7,\ell}(x) = -\frac{1}{105}x^7 + \frac{5}{192}x^6 - \frac{1}{15}x^5 + \frac{5}{32}x^4 - \frac{1}{3}x^3 + \frac{5}{8}x^2 - x + \frac{5}{4},$$
$$T_{8,u}(x) = \frac{47}{14400}\,x^8 - \frac{1}{105}x^7 + \frac{47}{1800}x^6 - \frac{1}{15}x^5 + \frac{47}{300}x^4 - \frac{1}{3}x^3 + \frac{47}{75}x^2 - x + \frac{94}{75},$$

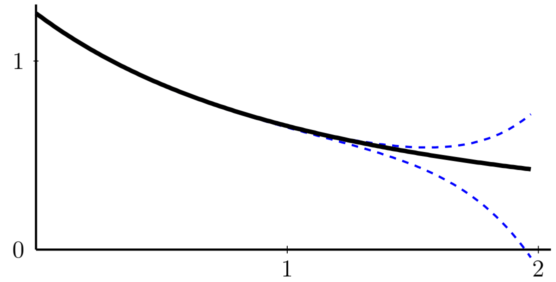

Figure 2. Solid line: function f. Upper and lower dashed lines: polynomials $T_{8,u}$ and $T_{7,\ell}$ respectively.

see Figure 2. We first check that $T_{7,\ell}(x) > 0$ for $x \in [0,1]$. This is done using that $T_{7,\ell}$ is a polynomial with rational coefficients, and thus its roots can be studied by finite algorithms. Specifically, by using Sturm Theorem (see the appendix), the number of real roots of such a polynomial in an interval with rational extremes, or in an infinite interval, can be computed. In the case of $T_{7,\ell}$ there are no real roots in the interval $[0,1]$; actually, the first positive real root can be located at the interval $(31/16, 2)$, as Figure 2 illustrates. Since $T_{7,\ell}(0) > 0$, it follows the strict positivity of $T_{7,\ell}$ on $[0,1]$.

Now, in the expression of $g(x)$, change $f(x)$ in the terms with positive sign by $T_{7,\ell}(x)$, and by $T_{8,u}(x)$ in the terms with negative sign. We get the polynomial

$$G(x) = 2 + x^2 T_{7,\ell}^2(x) - T_{8,u}^2(x) - 3x T_{8,u}(x),$$

which is

$$\begin{aligned} G(x) =& \frac{813359}{10160640000} x^{16} - \frac{41}{94500} x^{15} + \frac{17139569}{10160640000} x^{14} - \frac{139}{25200} x^{13} + \frac{1158121}{72576000} x^{12} \\ & - \frac{15671}{378000} x^{11} + \frac{1308953}{13440000} x^{10} - \frac{327233}{1512000} x^9 + \frac{1528967}{3780000} x^8 - \frac{9941}{14000} x^7 + \frac{616499}{540000} x^6 \\ & - \frac{1862}{1125} x^5 + \frac{189937}{90000} x^4 - \frac{1031}{450} x^3 + \frac{179249}{90000} x^2 - \frac{94}{75} x + \frac{2414}{5625}, \end{aligned}$$

and it satisfies

$$g(x) > G(x) > 0, \text{ for } x \in [0,1].$$

As before, the strict positivity of G on $[0,1]$ is proved observing that $G(0) > 0$, and that the polynomial G has no real roots in that interval; in fact G has exactly two real roots and the smallest one is in $(11/10, 12/10)$.

Notice that the trick of replacing $\sqrt{2\pi}$ by upper or lower rational bounds is crucial because it allows the use of the aforementioned approach.

Step 2. $x > 1$**.** By Proposition 8 we approximate f by $Q_{10}(x)/P_{10}(x) < f(x) < Q_{11}(x)/P_{11}(x)$, where

$$\frac{Q_{10}(x)}{P_{10}(x)} = \frac{x^9 + 44x^7 + 588x^5 + 2640x^3 + 2895x}{x^{10} + 45x^8 + 630x^6 + 3150x^4 + 4725x^2 + 945},$$

$$\frac{Q_{11}(x)}{P_{11}(x)} = \frac{x^{10} + 54x^8 + 938x^6 + 6090x^4 + 12645x^2 + 3840}{x^{11} + 55x^9 + 990x^7 + 6930x^5 + 17325x^3 + 10395x},$$

see Figure 3. Then in g change f by Q_{10}/P_{10} in the terms with positive signs, and by Q_{11}/P_{11} in the terms with negative sign. We obtain a rational function with positive denominator, and numerator

$$\begin{aligned} N(x) =& x^{36} + 185x^{34} + 15388x^{32} + 761580x^{30} + 25019940x^{28} + 576522420x^{26} \\ & + 9601604100x^{24} + 117398708820x^{22} + 1059855272550x^{20} + 7043405005350x^{18} \\ & + 33995881448100x^{16} + 115607852356500x^{14} + 259703297525700x^{12} \\ & + 329529066520500x^{10} + 108511796893500x^8 - 233411033740500x^6 \\ & - 247669566519375x^4 - 66176702274375x^2 - 6584094720000. \end{aligned}$$

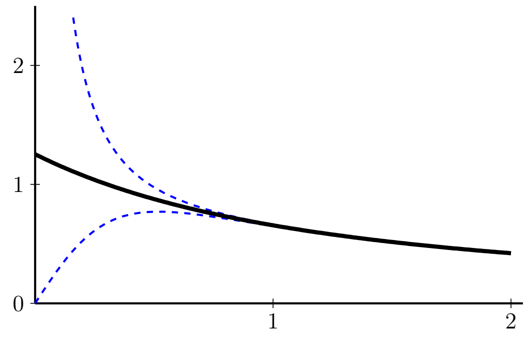

Figure 3. Solid line: function f. Upper and lower dashed lines: rational functions Q_{11}/P_{11} and Q_{10}/P_{10} respectively.

So it suffices to prove that $N(x) > 0$ for $x > 1$. This again is a consequence of the Sturm Theorem, which implies that N has no real roots in $(1, \infty)$ since its biggest root is in the interval $(93/100, 94/100)$, and $N(1) > 0$. $\square$

3.3 A second application: Bounds involving square roots

As a second application we study lower and upper bounds of f of the form

$$\psi_{a,b,c}(x) = \frac{a}{\sqrt{x^2+b}+cx}, \text{ with } a,\ b,\ c > 0. \tag{30}$$

The asymptotic expansion at infinity of such a function is

$$\psi_{a,b,c}(x) \sim \frac{\gamma_1}{x} + \frac{\gamma_3}{x^3} + \frac{\gamma_5}{x^5} + \cdots, \ x \to \infty, \tag{31}$$

for $\gamma_i = \gamma_i(a,b,c),\ i = 1, 3, \ldots$, which is of the same type of the expansion of f (see (7)). Well known bounds of this class are, for $x \geq 0$,

$$\frac{2}{\sqrt{x^2+4}+x} < f(x) < \frac{4}{\sqrt{x^2+8}+3x}. \tag{32}$$

The lower bound was proved by Birnbaum [4]; it is also given in Itô and McKean [16, Page 17], jointly with a worst upper bound, and attributed to Y. Komatu (1955) (see the reference therein). The upper bound is equivalent to the strict convexity of f (see the proof of Theorem 1), and, as we commented, it was proved by Sampford [29] and Shenton [31].

However, these bounds have at 0 different values than $f(0)$, and then Boyd [6] (reproduced in Mitrinović [23, p. 179]; see also Amos [1, Inequalities (12)]) gives the following new bounds, for $x > 0$,

$$\frac{\pi}{\sqrt{x^2+2\pi}+(\pi-1)x} < f(x) < \frac{\pi}{\sqrt{(\pi-2)^2x^2+2\pi}+2x}.$$

These bounds, denoted by $\underline{\psi}$ and $\overline{\psi}$ respectively, satisfy that

$$\underline{\psi}(0) = \overline{\psi}(0) = f(0) \quad \text{and} \quad \lim_{x\to\infty} x\big(\underline{\psi}(x) - f(x)\big) = \lim_{x\to\infty} x\big(\overline{\psi}(x) - f(x)\big) = 0,$$

and they are the sharpest bounds of the form $\psi_{a,b,c}$ that satisfy the above conditions.

To systematize and compare these bounds we introduce some notation: We will consider a generic function g that is enough regular at 0 an that have an asymptotic expansion at infinity as the one given in (31). We say the such a function g is equal to f at 0 of order $i \geq 1$ if g and f, and its derivatives up to order $i-1$ coincide at 0, that is,

$$g^{(k)}(0) = f^{(k)}(0), \text{for } k = 0, \ldots, i-1.$$

We say that g and f are equal at 0 of order 0 if there is no condition of the values of g and h (and its derivatives) at 0. In a similar way, we say that g and f are equal at infinity of order $j \geq 1$ if

$$\lim_{x\to\infty} x^k \left(g(x) - f(x)\right) = 0, \text{for } k = 0, \dots, 2j-1,$$

and that they are equal of order 0 if there is no restriction on the behaviour at infinity. Finally, for $i, j \geq 0$, we say that g and f are equal of order (i, j) if they are equal at 0 of order i and at infinity at order j.

Particularizing these notations to our bounds, since $\psi_{a,b,c}$ has three free parameters, we introduce four functions to study the different possibilities of equality between $\psi_{a,b,c}$ and f. For $i, j \in \{0, 1, 2, 3\}$ such that $i + j = 3$, we denote by $W_{i,j}$ the function $\psi_{a,b,c}$ which is equal to f of order (i, j). The four functions are

$$W_{3,0}(x) = \frac{\pi}{\sqrt{2x^2(4-\pi) + 2\pi} + 2x}, \quad W_{1,2}(x) = \frac{\pi}{\sqrt{x^2 + 2\pi} + (\pi - 1)x},$$

$$W_{2,1}(x) = \frac{\pi}{\sqrt{(\pi-2)^2 x^2 + 2\pi} + 2x} \quad \text{and} \quad W_{0,3}(x) = \frac{4}{\sqrt{x^2 + 8} + 3x}.$$

Note that $W_{1,2} = \underline{\psi}$ and $W_{2,1} = \overline{\psi}$, and $W_{0,3}$ coincides with the upper bound in (32). $W_{3,0}$ seems to be new. For the deduction of these functions see the proof of point 2 in the next theorem:

Theorem 10.

1. *For $x > 0$,*

$$\max\left\{W_{3,0}(x),\, W_{1,2}(x)\right\} < f(x) < \min\left\{W_{0,3}(x),\, W_{2,1}(x)\right\}.$$

2. *For $(i, j) = (0, 2)$ or $(i, j) = (2, 0)$, the functions $W_{i+1,j}$ and $W_{i,j+1}$ are the sharpest lower and upper bound of f of the form $\psi_{a,b,c}$ such that are equal to f of order (i, j). Moreover, the functions $W_{1,2}$ and $W_{2,1}$ are the sharpest lower and upper bound of f of the form $\psi_{a,b,c}$ such that are equal to f of order $(1, 1)$*

3. *Between the possible combination of upper and lower bounds, $W_{2,1}$ and $W_{3,0}$ are optimal in the sense that $\max_{x\geq 0} \left(W_{2,1}(x) - W_{3,0}(x)\right)$ is minimal. In particular,*

$$\max_{x\geq 0} \Big(W_{2,1}(x) - W_{3,0}(x)\Big) < 0.015.$$

Proof.
1. We always assume $x > 0$. This part refers to four inequalities. As we already commented, $f(x) < W_{0,3}(x)$ is equivalent to

$$2 + x^2 f^2(x) - f^2(x) - 3xf(x) > 0$$

and we proved it in Theorem 1. We now prove $W_{3,0}(x) < f(x)$, which is new, and we omit the proofs of the other two inequalities, that are very similar (and, indeed, these bounds are known).

The inequality $W_{3,0}(x) < f(x)$ is equivalent to

$$4x^2 f^2(x) - 2\pi x^2 f^2(x) + 2\pi f^2(x) + 4\pi x f(x) - \pi^2 > 0. \tag{33}$$

The main difficulty in this proof is the apparition of π and π^2 in the above inequality, and it is not convenient to change these number by rational approximations till the last moment. The proof has two steps:

First step: $x \in (0, 1]$. We will use the Taylor polynomials T_7 and T_8 as in the proof of Theorem 1. Specifically, in the left hand side of (33) change f by T_7 in positive terms and by T_8 in the negative terms. We get a polynomial of degree 18 where some coefficients are multiplied by $\sqrt{\pi/2}$, $\sqrt{2/\pi}$, π or $1/\pi$. Now in the terms with $\sqrt{\pi/2}$, $\sqrt{2/\pi}$ change them by fractions (in agreement with the sign) by using the convergents of $\sqrt{\pi/2}$ given by

$$\frac{851}{679} < \sqrt{\frac{\pi}{2}} < \frac{94}{75}, \tag{34}$$

and finally, change π and $1/\pi$ by using

$$\frac{333}{106} < \pi < \frac{355}{113}. \tag{35}$$

We get a polynomial with rational coefficients that by Sturm Theorem is strictly positive in $(0, 1]$.

Second step: $x > 1$. In the expression of the left hand side of (33), first substitute f in the positive terms by Q_{12}/P_{12} and in the negative terms by Q_{13}/P_{13}. This gives a rational function with positive denominator. The numerator is a polynomial of order 48 with integer coefficients some of them multiplied by π or π^2. In that expression, use the convergents of π given in (35). We arrive to a polynomial with rational coefficients that, by Sturm Theorem, is strictly positive for $x > 1$.

2. We prove that $W_{3,0}$ and $W_{2,1}$ are the sharpest upper and lower bounds of f of the form $\psi_{a,b,c}$ such that are equal to f of order $(2, 0)$. Later, we comment the proofs of the other cases.

First we consider the family of functions $\psi_{a,b,c}$ such that are equal to f of order $(2, 0)$. From $f(0) = \sqrt{\pi/2}$ and $f'(0) = -1$ we deduce that $a = \pi c/2$ and $b = \pi c^2/2$. Hence we can parametrize that family by

$$\psi_c(x) = \frac{\pi c/2}{\sqrt{x^2 + \pi c^2/2 + cx}},\ c > 0.$$

Fixed $x > 0$, by derivation with respect to c, it is proven that the function $c \in (0, \infty) \to \psi_c(x)$ is strictly increasing. Hence, for the optimal lower bound we should take c as large as possible satisfying $\psi_c(x) < f(x)$, and for the optimal upper bound, c as small as possible with $f(x) < \psi_c(x)$.

Imposing that ψ_c is equal to f of order $(3, 0)$, that means, $\psi_c''(0) = f''(0) = \sqrt{\pi/2}$, we deduce that c should be $c_0 = \sqrt{2/(4 - \pi)}$. Note that $\psi_{c_0} = W_{3,0}$. On the other hand, to look c such that ψ_c is equal to f of order (2,1), consider the asymptotic expansion of ψ_c when $x \to \infty$,

$$\psi_c(x) \sim \frac{\pi c}{2 + 2c}\frac{1}{x} + \cdots .$$

Comparing with the asymptotic expansion of f (see (7)) we should take $c_1 = 2/(\pi - 2)$. Then $\psi_{c_1} = W_{2,1}$. Note that $c_0 < c_1$.

By Taylor formula for ψ_c it is deduced that

$$\lim_{x\to 0} \frac{f(x) - \psi_c(x)}{x^2} = \frac{(\pi - 4)c^2 + 2}{2\sqrt{2\pi}c^2}.$$

Hence, if $c > c_0$, that limit is negative, and then, for x near 0, $f(x) < \psi_c(x)$. So ψ_c is not a lower bond.

Now, from the asymptotic expansion when $x \to \infty$ of ψ_c and f it follows that

$$\lim_{x\to\infty} x\big(f(x) - \psi_c(x)\big) = \frac{(2 - \pi)c + 2}{2 + 2c}.$$

Then, if $c < c_1$, we have that for x large enough, $f(x) > \psi_c(x)$, so ψ_c is not an upper bound.

To summarize, by point **1**, $\psi_{c_0}(x) < f(x) < \psi_{c_1}(x)$, and for $c \in (c_0, c_1)$, ψ_c is neither a lower bound nor an upper bound, Then the proof is complete.

For the case $W_{1,2}$ and $W_{1,3}$, the functions $\psi_{a,b,c}$ such that has a coincidence of order (1,1) with f can be parametrized as

$$\eta_a(x) = \frac{a}{\sqrt{x^2 + 2a^2/\pi + (a - 1)x}},\ a > 1. \tag{36}$$

The function $W_{1,2}$ is the case $a_0 = \pi$, and $W_{2,1}$ is $a_1 = \pi/(\pi - 2)$. Fixed $x > 0$, The function $a \to \eta_a(x)$ is strictly decreasing, and for $a \in \big(\pi/(2 - \pi), \pi\big)$, the function η_a is neither a lower bound nor an upper bound.

Finally, consider the case $W_{1,2}$ and $W_{0,3}$. The functions $\psi_{a,b,c}$ such that has a coincidence of order (0,2) with f can be parametrized as

$$\chi_c(x) = \frac{1 + c}{\sqrt{x^2 + 2(1 + c) + cx}}. \tag{37}$$

The function χ_c with a coincidence of order (1,2) with f corresponds to $c = \pi - 1$, and it is $W_{1,2}$. The function χ_c with a coincidence of order (0,3) with f corresponds to $c = 3$ and it is $W_{0,3}$. Using a similar argument it is proved that for $c \in (\pi - 1, 3)$, ψ_c is neither a lower bound nor an upper bound.

3. We first will prove that $\sup_{x\geq 0}\big(W_{2,1}(x) - W_{3,0}(x)\big) < 0.015$. To this end, write $W(x) = W_{2,1}(x) - W_{3,0}(x)$,

$$W_{2,1}(x) = \frac{\pi}{\sqrt{(\pi-2)^2x^2 + 2\pi} + 2x} = \frac{\pi}{\Delta_0(x) + 2x},$$

and

$$W_{3,0}(x) = \frac{\pi}{\sqrt{2x^2(4-\pi) + 2\pi} + 2x} = \frac{\pi}{\Delta_1(x) + 2x},$$

A computation shows that

$$W'(x) = \frac{\pi x M(x)}{\Delta_0(x)\Delta_1(x)\big(\Delta_0(x) + 2x\big)^2\big(\Delta_1(x) + 2x\big)^2},$$

where $M(x)$ is a polynomial. So the zeroes of $M(x)$ will give the behaviour of W. Squaring conveniently the equation $M(x) = 0$, which includes radicals, it can be translated to a polynomial equation and we have that if x_0 is a zero of M then it is also a zero of a certain polynomial say, R_{12} (the reciprocal is not true); that polynomial has the form

$$R_{12}(x) = a_6x^{12} + a_5x^{10} + a_4x^8 + a_3x^6 + a_2x^4 + a_1x^2 + a_0,$$

where $a_6, a_5, a_4, a_3, a_0 > 0$ and $a_2, a_1 < 0$. By Descartes Theorem, R_{12} will have two positive zeroes or none. Moreover, $R_{12}(0) > 0,\ R_{12}(17/10) < 0,\ R_{12}(\infty) > 0$, and by Bolzano theorem R_{12} has exactly two real zeroes, say x_1 and x_2. Moreover,

$$R_{12}(15/10)R_{12}(16/10) < 0 \quad \text{and} \quad R_{12}(198/100)R_{12}(199/100) < 0,$$

and

$$M(1) > 0,\ M(17/10) > 0 \quad \text{and} \quad M(2) < 0.$$

This implies that x_1 is not a zero of M (x_1 is a spurious zero introduced by the procedure to cancel the radicals). To summarize, W has a maximum at $x_2 \in I := (198/100, 199/100)$. Finally, both $W_{2,1}$ and $W_{3,0}$ are strictly decreasing, so

$$\max_{x\geq 0}\Big(W_{2,1}(x) - W_{3,0}(x)\Big) = \max_{x\in I}\Big(W_{2,1}(x) - W_{3,0}(x)\Big) \leq W_{2,1}(198/100) - W_{3,0}(199/100) < 0.015.$$

Now it is easy to check that there are $y_1, y_2, y_3 \geq 0$ such that $W_{2,1}(y_1) - W_{1,2}(y_1) > 0.015$, $W_{0,3}(y_2) - W_{1,2}(y_2) > 0.015$ and $W_{0,3}(y_3) - W_{3.0}(y_3) > 0.015$.

□

Remarks 11.

1. Note that from the expression (36) and the properties of the function η_a, taking $a = 2$ we get a nice and simple upper bound of f. Specifically,

$$\eta_2(x) = \frac{2}{\sqrt{x^2 + 8/\pi} + x}.$$

This bound was found by Pollak [26] (see also Mitrinović [23, p. 179]).

2. In a similar way, from the expression (37) a lower bound for f, less sharp than $W_{1,2}$, but more friendly, is given by taking $c = 2$, which gives

$$\chi_2(x) = \frac{3}{\sqrt{x^2+6}+2x}.$$

3. The three parameters of $\psi_{a,b,c}$ allow to build alternative bounds adapted to more specific purposes. For example, we construct lower and upper bounds that approximate sharply f in a neighborhood of $x = 2$; they are based in a function with a coincidence with f of order (1,1) and later manipulating the coefficients in order that a, b, c to be rational numbers: for $x > 0$,

$$\frac{200}{\sqrt{1521x^2+25600}+161x} < f(x) < \frac{192}{\sqrt{4225x^2+20736}+127x}.$$

The proof is analogous to the proofs of the bounds in Theorem 10

3.4 More bounds with rational or exponential functions

The topic of searching new bounds for the Mills ratio seems inexhaustible, and we would like to mention the papers of Dümbgen [12] and Avram [2] where new methodologies are presented. To finish we study five families of bounds and we just emphatize that all inequalities are proved by the same method.

1. Padé approximations at the origin. In Corollary 2 we proved that the rational fractions Q_n/P_n are the Padé–Laurent approximations at infinity. Now we will consider Padé approximations at the origin. Standard computations show that (with the usual notations for Padé aproximations)

$$p_{0,1}(x) = \frac{\pi}{\sqrt{2\pi}+2x} \quad \text{and} \quad p_{1,2}(x) = \frac{6\pi\sqrt{2\pi}-24\sqrt{2\pi}+(48-16\pi)x}{12\pi-48-4\sqrt{2\pi}x+2(8-3\pi)x^2}.$$

Using our procedure, it is proven that for $x > 0$,

$$p_{1,2}(x) < f(x) < p_{0,1}(x).$$

It is worth to comment that $p_{0,1}(x)$ is very simple and it is a good global approximation to f. Actually, $p_{0,1}(x) - p_{1,2}(x) < 0.08$

2. Bounds with simple rational functions. We construct bounds of the type $a/(b+x)$. Note that such functions have an expansion at infinity with nonzero terms in the even coefficients, so we need to change slightly our notations of Section 3.3; here and in next points, we say that g is equal to f at infinity of order $j \geq 1$ if $\lim_{x\to\infty} x^k\big(g(x) - f(x)\big) = 0$ for $k = 0, \dots, j$ (the notation for the equality at 0 does need to be modified). We consider only the most interesting cases. Let $U_{2,0}$ equal to f of order (2,0) and $U_{1,1}$ equal of order (1,1). They are

$$U_{2,0}(x) = \frac{\pi}{\sqrt{2\pi}+2x} \quad \text{and} \quad U_{1,1}(x) = \frac{\pi}{\sqrt{2\pi}+\pi x}.$$

Note that $U_{2,0} = p_{0,1}$ of previous point. We consider also approximations to both function with rational coefficients. It is proved that for $x > 0$,

$$\frac{105}{91+110x} < U_{1,1}(x) < f(x) < U_{2,0}(x) < \frac{44}{35+28x}.$$

We have that $U_{2,0}(x) - U_{1,1}(x) < 0.15$, and the difference between the corresponding bounds with rational coefficients is lower than 0.19.

3. Bounds with quadratic rational functions. Following an idea of Bryc [7] we consider functions of the form $V(x) = (a+bx)/(c+dx+x^2)$. We study some of the functions $V_{i,j}$ with $i+j = 4$ such that are equal to

f of order (i,j). First we consider the functions $V_{2,2}$ and $V_{1,3}$, and some corresponding functions with simple rational coefficients. We have

$$\frac{35+15x}{28+37x+16x^2} < V_{2,2}(x) = \frac{\sqrt{2\pi}+(\pi-2)x}{2+x\sqrt{2\pi}+(\pi-2)x^2} < f(x)$$
$$< V_{1,3}(x) = \frac{\sqrt{2\pi}+2x}{2+x\sqrt{2\pi}+2x^2} < \frac{2}{5}\,\frac{13+10x}{4+5x+4x^2}.$$

The bounds are quite good: $V_{1,3}(x) - V_{2,2}(x) < 0.07$, and the difference between the corresponding bounds with rational coefficients is lower than 0.13.

The function $V_{3,1}$ is also interesting. Its expression is

$$V_{3,1}(x) = \frac{\sqrt{2\pi}(\pi-2)+(4-\pi)x}{2(\pi-2)+\sqrt{2\pi}x+(4-\pi)x^2}.$$

It is given in Bryc [7] (see also Avram [2]) as a good uniform approximation to f without a formal proof. Following our procedure it is proven that it is an upper bound of f, and indeed better than $V_{1,3}$ since $V_{3,1}(x) - V_{2,2}(x) < 0.015$.

4. Bounds involving one exponential term. Inspired by Karagiannidis and Lioumpas [17] we consider upper and lower bounds of f of the form

$$\kappa_{a,b}(x) = \frac{1-e^{-ax}}{bx},$$

for $a,b>0$. In Karagiannidis and Lioumpas [17] the values $\bar{a} = 1.98/\sqrt{2}$ and $\bar{b} = 1.135$ are proposed to get a good approximation to f based on numerical arguments. Following the notations introduced at point **2** we consider the functions $Z_{2,0}$ and $Z_{1,1}$ given by

$$Z_{2,0}(x) = \frac{1-e^{-4x/\sqrt{2\pi}}}{4x/\pi} \quad \text{and} \quad Z_{1,1}(x) = \frac{1-e^{-\sqrt{2\pi}\,x/2}}{x}.$$

Combining the approximations of f with the properties of a function of the form $1-\exp(-ax)$, the study of inequalities between f and $\kappa_{a,b}$ are reduced to prove the strict positivity of certain polynomials with rational coefficients, as in the previous sections. It is proved that for $x>0$,

$$Z_{2,0}(x) < f(x) < Z_{1,1}(x).$$

These bounds are quite good since $Z_{1,1}(x) - Z_{2,0}(x) < 0.1$. Moreover, following the same arguments as in Theorem 10 it is proved that $Z_{2,0}$ and $Z_{1,1}$ are the sharpest lower and upper bound of the form $\kappa_{a,b}$ such that $\lim_{x\to 0}\kappa_{a,b}(x) = f(0)$. The function $\kappa_{\bar{a},\bar{b}}$ proposed by Karagiannidis and Lioumpas [17] is neither a lower bound nor an upper bound.

5. Chernoff type bounds for the Gaussian Q-function. In the engineering literature the function

$$Q(x) = \frac{1}{\sqrt{2\pi}}\int_x^\infty e^{-t^2/2}\,dt$$

is called the Gaussian Q–function. By technical reasons (see Chang *et al.* [8] and Côté *et al.* [10] and the references therein), Chernoff type bounds for Q of the form

$$C_{a,b}(x) = a\,e^{-bx^2},\ x \ge 0,$$

for $a,\ b \ge 0$, are particulary convenient in the analysis of communications systems. Since

$$Q(x) = \frac{1}{\sqrt{2\pi}}\,e^{-x^2/2}f(x),$$

Chernoff type bounds for Mills ratio give automatically Chernoff type bounds for Q. In particular, for $x > 0$,

$$e^{-3x^2/5} < f(x) < \sqrt{\frac{\pi}{2}}.$$

Hence,

$$\frac{1}{\sqrt{2\pi}} e^{-11x^2/10} < Q(x) < \frac{1}{2} e^{-x^2/2}.$$

The upper bound follows from the fact that f is strictly decreasing and $f(0) = \sqrt{\pi/2}$; in agreement with Chang *et al.* [8, Corollary 1] it is the optimal Chernoff type upper bound for Q. The lower bound is proved applying our procedure.

Appendix: Sturm Theorem

We present a general version of Sturm Theorem [33] (see Isaacson and Keller [15, Page 126]). Let $f : [a, b] \to \mathbb{R}$ be a differentiable function. A sequence of continuous functions on $[a, b]$, $\{f_0, f_1, ..., f_m\}$, with $f_0 = f$, is called a Sturm sequence for f on $[a, b]$ if the following holds:

1. f has at most simple roots in $[a, b]$.

2. f_m does not vanish in $[a, b]$.

3. If $f(x_0) = 0$ for some $x_0 \in [a, b]$ then $f_1(x_0)f_0'(x_0) > 0$.

4. If for some $i > 0$, $f_i(x_0) = 0$ with $x_0 \in [a, b]$ then $f_{i+1}(x_0)f_{i-1}(x_0) < 0$.

Sturm Theorem. *Let $\{f_0, f_1, ..., f_m\}$ be a Sturm sequence for $f = f_0$ on $[a, b]$ with $f(a)f(b) \neq 0$. Then the number of solutions of $f = 0$ on (a, b) is equal to $V(a) - V(b)$, where $V(c)$ is the number of changes of sign in the sequence $[f_0(c), f_1(c), \ldots, f_m(c)]$.*

We remark that if in $[f_0(c), f_1(c), \ldots, f_m(c)]$ some value $f_j(c)$ vanishes, then it does not contribute to the number of changes of sign of the sequence.

When f is a polynomial, Sturm approach enjoys the very useful properties that it can be applied even without knowing a priori if the polynomial has simple roots, and that there is a simple procedure to construct its Sturm sequence. Indeed, if p is a polynomial of degree n then define $\{p_0, p_1, ..., p_m\}$ with $m \leq n$ setting $p_0 = p$, $p_1 = p'$ and

$$\begin{aligned} p_{i-1}(x) &= q_i(x)p_i(x) - p_{i+1}(x), \quad \text{for} \quad i = 1, 2, \ldots, 2, \ldots, m-1, \\ p_{m-1}(x) &= q_m(x)p_m(x), \end{aligned}$$

where q_i and p_{i+1} are respectively the quotient and the remainder (the latter with the sign changed) of the division of p_{i-1} by p_i. The construction of this sequence ends when the remainder is zero, i.e., $p_{m+1} = 0$. In this case, since this procedure is essentially the Euclides algorithm, p_m is the greatest common divisor of p_0 and p_1. When all the zeros of p are simple then $m = n$ and p_m is a nonzero constant. Then it is easy to show that $\{p_0, p_1, ..., p_m\}$ is a Sturm sequence for p on any interval. If p has some multiple zeroes then $m < n$. Since p_m divides both p_0 and p_1, it also divides p_i for all i. Then setting $\widetilde{p}_i = p_i/p_m$, it happens that $\widetilde{p}_0$ has the same zeroes of p but all with multiplicity 1, and $\{\widetilde{p}_0, \widetilde{p}_1, ..., \widetilde{p}_m\}$ is a Sturm sequence for $\widetilde{p}_0$ on any interval, and so the localizacion problem of the real zeroes of p is solved.

In the particular case that the polynomial p has rational coefficients and a and b are also in $\mathbb{Q}$ then all the conditions of Sturm Theorem can be checked analytically. Clearly, this result can be extended to $a = -\infty$ or $b = \infty$.

As an illustration of the method we give all the details for proving that the function g appearing in the proof of Theorem 9 is strictly positive in $[0, 45/100]$. We have that for $x \in [0, 45/100]$,

$$0 < -x + \frac{5}{4} = T_{1,\ell}(x) < T_1(x) < f(x) < T_2(x) < T_{2,u}(x) = \frac{47}{75}x^2 - x + \frac{94}{75}.$$

Define the polynomial

$$p(x) = 2 + x^2 T_{1,\ell}^2(x) - T_{2,u}^2(x) - 3xT_{2,u}(x),$$

which satisfies that $p(x) < g(x)$ for $x \in [0, 45/100]$. Then

$$p(x) = p_0(x) = \frac{3416}{5625}x^4 - \frac{469}{150}x^3 + \frac{179249}{90000}x^2 - \frac{94}{75}x + \frac{2414}{5625}.$$

Its Sturm sequence is

$$\begin{aligned}
p_1(x) &= \frac{13664}{5625}x^3 - \frac{469}{50}x^2 + \frac{179249}{45000}x - \frac{94}{75}, \\
p_2(x) &= \frac{355316101}{175680000}x^2 - \frac{3202259}{9369600}x - \frac{1135387}{43920000}, \\
p_3(x) &= -\frac{45065042306901196}{18035647375691743}x + \frac{24672388276565440}{18035647375691743}, \\
p_4(x) &= -\frac{245489329508793336223961143932017 47}{624239151062334427060084458882300 00}.
\end{aligned}$$

Define $S(c) = [\mathrm{sgn}(p_0(c)), \mathrm{sgn}(p_1(c)), \ldots, \mathrm{sgn}(p_4(c))]$, with $c \in \mathbb{R} \cup \{-\infty, \infty\}$, where by notation $\mathrm{sgn}(\pm\infty) = \pm$.

It holds that $S(0) = [+, -, -, +, -]$, $S(45/100) = [+, -, +, +, -]$, $S(46/100) = [-, -, +, +, -]$ and $S(+\infty) = [+, +, +, -, -]$. Hence $V(0) = 3$, $V(45/100) = 3$, $V(46/100) = 2$ and $V(+\infty) = 1$. By Sturm Theorem we deduce that p has $V(0) - V(45/100) = 0$ real roots in $(0, 45/100)$. Moreover p has exactly $V(0) - V(+\infty) = 2$ positive real roots and the smallest one is in $(45/100, 46/100)$. Hence, since $p(0) > 0$, it holds that $g(x) > p(x) > 0$ on $[0, 45/100]$, as we wanted to prove.

Notice that the proofs of Steps 1 and 2 in Theorem 9 follow the same ideas but involve much more computations which, for the sake of simplicity, are omitted. In that proofs we used Maple software to do the computations.

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