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Uniform (very) sharp bounds for ratios of parabolic cylinder functions

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Abstract

Parabolic cylinder functions are classical special functions with applications in many different fields. However, there is little information available regarding simple uniform approximations and bounds for these functions. We obtain very sharp bounds for the ratio $\Phi_n(x) = U(n-1,x)/U(n,x)$ and the double ratio $\Phi_n(x)/\Phi_{n+1}(x)$ in terms of elementary functions (algebraic or trigonometric) and prove the monotonicity of these ratios; bounds for $U(n,z)/U(n,y)$ are also made available. The bounds are very sharp as $x \to \pm\infty$ and $n \to +\infty$, and this simultaneous sharpness in three different directions explains their remarkable global accuracy. Upper and lower elementary bounds are obtained which are able to produce several digits of accuracy for moderately large $|x|$ and/or n.

KEYWORDS

approximations and bounds, asymptotic analysis, numerical methods, parabolic cylinder functions, special functions

1 | INTRODUCTION

Parabolic cylinder functions (PCFs), solutions of the second-order ODE

$$y''(x) - \left(\frac{x^2}{4} + n\right) y(x) = 0, \tag{1}$$

are classical special functions (with Hermite functions as a particular case) which find applications in many scientific fields. In particular, the ratios of the recessive solution as $x \to +\infty$, $U(n, x)$, appear in probabilistic contexts, for example, as moments of certain distributions (see Ref. [1] for an application in crystallography) and in the analysis of Ornstein–Uhlenbeck and Lévy processes[2,3] and their applications in finance,[4] neurobiology,[5] and statistical physics,[6] among other examples.

Despite their relevance, little is known regarding simple functional uniform approximations and bounds,[7,8] which is in contrast to the vast information available on other functions like, for instance, modified Bessel functions (see Refs. [9–12] and references cited therein). Recently, one new monotonicity property was discovered for ratios of the PCFs from stochastic considerations[7] that had not been proved by purely analytical methods before; this fact illustrates that there is a clear deficit in the amount of analytical information on these functions.

Here we propose to invert the process and to advance new properties, which supersede previous knowledge, using only basic analytical information, without recourse to more indirect arguments. We will not only prove the monotonicity property described in Ref. [7], but we will obtain from this analysis new and very sharp bounds for ratios of the PCFs.

In particular, we will obtain lower and upper bounds for the ratio $\Phi_n(x) = U(n-1, x)/U(n, x)$ that are very sharp in three different directions: $x \to \pm\infty$ and $n \to +\infty$. They are so sharp that, for instance, some of the bounds will display relative accuracies of order $\mathcal{O}(x^{-6})$ as $x \to +\infty$, $\mathcal{O}(x^{-4})$ as $x \to -\infty$, and $\mathcal{O}(n^{-2})$ as $n \to +\infty$[1]. The bounds are, in fact, tight enough to give an accurate estimation of $\Phi_n(x)$ for moderate $|x|$ and n by using a very simple expression in terms of elementary functions (trigonometric or algebraic). It is expected that these approximations will play a role in future numerical algorithms for computing these special functions, in particular for improving the performance of the evaluation of $U(n, x)$ by backward recurrence and continued fraction evaluations.[13,14]

The techniques employed will be related to those considered for modified Bessel functions in Ref. [12] and later generalized in Ref. [8] (with application to the PCFs), but they will go far beyond the possibilities of the analysis of Riccati equations presented in those papers, and they offer a new method for obtaining accurate information on the ratios of a large number of special functions.

The structure of the paper is as follows: In Section 2, we give the basic analytical information we will need of the PCF $U(n, x)$. In Section 3, we briefly summarize the results in Ref. [8]; this will set the starting point and it will provide some necessary information for the next step. In addition, the results of this section will suggest a very sharp bound for the double ratio $\Phi_n(x)/\Phi_{n+1}(x)$ which we will be able to prove in Section 4. In Section 4, we discuss the new method and we will prove that the new results (of trigonometric or algebraic form) supersede previous results in all aspects. We prove the monotonicity of the ratio $\Phi_n(x)$ and the double ratio $\Phi_n(x)/\Phi_{n+1}(x)$ and obtain very sharp bounds for both ratios, from where bounds for the ratios $U(n, z)/U(n, y)$ can also be obtained (and then bounds on $U(n, z)$ become available because $U(n, 0)$ is known). Finally, we illustrate numerically the sharpness of these bounds in Section 5.

2 | PROPERTIES OF THE FUNCTION $U(n, x)$

To prove all the monotonicity properties and bounds in this paper, we will only need the following three pieces of information:

[1] If the bound had relative error $\mathcal{O}(x^{-1})$ we would already say that it is sharp; then, we can say that our bounds are very sharp in three different directions, and even extremely sharp as $|x| \to +\infty$.

1. The PCF $U(n,x)$ satisfies the following difference-differential system (see 12.8.2 and 12.8.3 of Ref. [15]):

$$U'(n,x) = \frac{x}{2}U(n,x) - U(n-1,x),$$
$$U'(n-1,x) = -\frac{x}{2}U(n-1,x) - (n-1/2)U(n,x), \tag{2}$$

and, as a consequence, they satisfy the three-term recurrence relation

$$(n+1/2)U(n+1,x) + xU(n,x) - U(n-1,x) = 0. \tag{3}$$

2. As $x \to +\infty$, the function

$$\Phi_n(x) = \frac{U(n-1,x)}{U(n,x)} \tag{4}$$

is positive and increasing when $n > 1/2$.
3. As $x \to +\infty$, the function

$$W_n(x) = \left(n + \frac{1}{2}\right)\frac{\Phi_n(x)}{\Phi_{n+1}(x)} = \left(n + \frac{1}{2}\right)\frac{U(n+1,x)U(n-1,x)}{U(n,x)^2} \tag{5}$$

is positive and increasing when $n > 1/2$ (the factor $n + 1/2$ is introduced for later convenience).

As we see, the required properties are very few, and the ideas should be easily applicable to a wide range of functions described in Ref. [8], that is, for solutions of monotonic difference-differential linear systems. We will explore this in future papers.

The properties as $x \to +\infty$ are easy to check from the asymptotic expansions of $U(n,x)$ [Ref. 15, 12.9.1]:

$$U(n,x) \sim e^{-x^2/4}x^{-n-1/2}\sum_{s=0}^{\infty}(-1)^s\frac{\left(\frac{1}{2}+n\right)_{2s}}{s!(2x^2)^s}, \quad x \to +\infty. \tag{6}$$

This expansion will also be useful for analyzing the sharpness of the bounds as $x \to +\infty$. Similarly, for analyzing the sharpness of the bounds as $x \to -\infty$ we use the expansion [Ref. 16, 11.2.23]:

$$U(n,x) \sim \frac{\sqrt{2\pi}e^{x^2/4}(-x)^{n-1/2}}{\Gamma\left(\frac{1}{2}+a\right)}\sum_{s=0}^{\infty}\frac{\left(\frac{1}{2}-n\right)_{2s}}{s!(2x^2)^s}, \quad x \to -\infty. \tag{7}$$

Using (6), we see that as $x \to +\infty$,

$$\Phi_n(x) \sim x[1 + (n+1/2)x^{-2} - (n+1/2)(n+3/2)x^4 + \mathcal{O}(x^{-6})], \tag{8}$$

and the first term is enough to see that, indeed, $\Phi_n(x)$ is positive and increasing as $x \to +\infty$.

Now from (7) we have, as $x \to -\infty$,

$$\Phi_n(x) \sim -\frac{n-1/2}{x}[1-(n-3/2)x^{-2}+2(n-3/2)(n-2)x^4+\mathcal{O}(x^{-6})]. \tag{9}$$

Also, combining (6) and (7)

$$W_n(x) \sim (n \pm 1/2)\left(1 \mp x^{-2} + \left(\frac{9}{2} \pm 3n\right)x^{-4} + \mathcal{O}(x^{-6})\right), \quad x \to \pm\infty, \tag{10}$$

and therefore $W_n(x)$ is increasing and positive as $x \to +\infty$, as announced.

3 | BOUNDS FROM THE RICCATI EQUATION AND THE RECURRENCE RELATION

We start this section by briefly summarizing some of the bounds that were obtained in Ref. [8], two of them rediscovered in Ref. 7. We prove them in a more straightforward way than in Ref. [8], and we use this to motivate the more accurate methods to be described later. In addition, we provide information on the sharpness of the bounds, to be compared with the new and tighter bounds of Section 4. Finally, a new (very sharp) bound is motivated by the bounds in this section, which we will be able to prove true in Section 4.

From (2), we deduce that $\Phi_n(x) = U(n-1,x)/U(n,x)$ satisfies

$$\Phi_n'(x) = \Phi_n(x)^2 - x\Phi_n(x) - (n-1/2). \tag{11}$$

Therefore, $\Phi_n(x)$ is one of the solutions of the Ricatti equation

$$y'(x) = y(x)^2 - xy(x) - (n-1/2).$$

In our analysis, the nullclines of the differential equations play a major role; these are the curves where $y'(x) = 0$. We will use the following lemma, which is immediate to prove with graphical arguments.

Lemma 1. *Let $y(x)$ be a solution of $y'(x) = y(x)^2 - xy(x) - a$, $a > 0$, such that $y(+\infty) > 0$ and $y'(+\infty) > 0$, then $y'(x) > 0$ and $y(x) > \lambda_+(x)$ for all $x \in \mathbb{R}$, where $\lambda_+(x) = (x + \sqrt{x^2+4a})/2$ is the positive nullcline of the Riccati equation.*

Proof. The nullclines of the Riccati equation are $\lambda_\pm(x)$, with $\lambda_+(x) = (x + \sqrt{x^2+4a})/2$ and $\lambda_-(x) = -\lambda_+(-x)$ and then $y'(x) = (y(x)-\lambda_+(x))(y(x)-\lambda_-(x))$; and because $y(+\infty) > 0$ and $y'(+\infty) > 0$ necessarily $y(x) > \lambda_+(x)$ for large enough x.

However then, because $\lambda_+'(x) > 0$ for all x, we have that $y(x) > \lambda_+(x)$ for all real x. In other to see this, we can follow the graph of $y(x)$ starting from a large enough value of x, x_∞, such that $y(x_\infty) > \lambda_+(x_\infty)$ and following the curve in the direction of decreasing x as described next.

In the first place, it is not possible that a value $x_c < x_\infty$ exists such that $y(x_c) = \lambda_+(x_c)$ (and then $y'(x_c) = 0$) starting from $y(x_\infty) > \lambda_+(x_\infty)$, because we would be approaching the nullcline from above and then $y'(x_c)$ should be larger than $\lambda_+'(x_c) > 0$, and there is a contradiction. On the other hand $y(x)$ stays finite for all real x (and continuous and differentiable): as said it cannot cross the nullcline and the only possibility would be to go to $+\infty$ for some $x_p < x_\infty$ but this is not possible because as long as $y(x) > \lambda_+(x)$ we have that $y'(x) > 0$ and therefore the values of $y(x)$ decrease as x decreases. ■

Theorem 1. *For all real x and $n > 1/2$, the ratio $\Phi_n(x) = U(n-1,x)/U(n,x)$ is increasing as a function of x and*

$$\Phi_n(x) > \frac{1}{2}\left(x + \sqrt{x^2 + 4n - 2}\right). \tag{12}$$

Proof. Considering (6) we have that $\Phi_n(x) = x(1 + \mathcal{O}(x^{-2}))$ as $x \to +\infty$. Therefore, $\phi_n(x)$ satisfies the hypotheses of Lemma 1 with $a = n - 1/2$. ■

Remark 1. Considering (8) and (9), we conclude that the bound is sharp both as $x \to \pm\infty$, as the first term in the expansion as $x \to \pm\infty$ coincides. It is, in fact, the only bound of the type $\alpha x + \sqrt{\beta x^2 + \gamma}$ satisfying these conditions, and in this sense it is the best possible lower bound.

Remark 2. All the bounds in this paper are sharp as $n \to +\infty$. See Section 5 for details.

Now we obtain two upper bounds combining the previous result with the use of the recurrence relation (3)

Corollary 1. *For $n > -1/2$ and all real x,*

$$\Phi_n(x) < \frac{1}{2}\left(x + \sqrt{x^2 + 4n + 2}\right). \tag{13}$$

Proof. We write the recurrence relation (3) in terms of $\Phi_n(x)$ as follows (backward recurrence):

$$\Phi_n(x) = x + (n + 1/2)/\Phi_{n+1}(x). \tag{14}$$

Now using Theorem 1 for $\Phi_{n+1}(x)$ we obtain the bound. ■

Remark 3. Care must be taken when using this to write a lower bound for $\Phi_n(x)^{-1} = U(n,x)/U(n-1,x)$, for $n \in (-1/2, 1/2)$ because in this case $\Phi_n(x)$ becomes negative for negative x.

Remark 4. The bound (13) is sharp as $x \to +\infty$ and the first two terms in the expansion (6) are reproduced. Contrarily, the bound is not sharp as $x \to -\infty$, as it gives $-(n + 1/2)/x + \mathcal{O}(x^{-3})$. It is, however, the bound of the form $\alpha x + \sqrt{\beta x^2 + \gamma}$ with the highest order of approximation as $x \to +\infty$ and such that it is $\mathcal{O}(x^{-1})$ as $x \to -\infty$.

Corollary 2. *For $n > 3/2$ and all real x,*

$$\Phi_n(x) < \frac{1}{2}\frac{n - 1/2}{n - 3/2}\left(x + \sqrt{x^2 + 4n - 6}\right). \tag{15}$$

Proof. We rewrite the three-term recurrence relation as (forward recurrence)

$$\Phi_n(x) = \frac{n-1/2}{-x+\Phi_{n-1}(x)}, \tag{16}$$

and apply Theorem 1 to $\Phi_{n-1}(x)$. ■

Remark 5. The bound (13) is sharp as $x \to -\infty$ and the first two terms in the expansion (6) are reproduced. Contrarily, the bound is not sharp as $x \to +\infty$, as it gives $x(n-1/2)/(n+3/2) + \mathcal{O}(x^{-1})$. It is, however, the bound of the form $\alpha x + \sqrt{\beta x^2 + \gamma}$ with the highest order of approximation as $x \to -\infty$ and such than it is $\mathcal{O}(x)$ as $x \to +\infty$.

The previous inequalities can be combined to obtain bounds for the double ratio $W_n(x) = (n + 1/2)\Phi_n(x)/\Phi_{n+1}(x)$. It is convenient to define

$$h_{\alpha,\beta}(x) = (n-\beta)\frac{x+\sqrt{4(n-\alpha)+x^2}}{x+\sqrt{4(n-\beta)+x^2}},$$

which satisfies $h_{\alpha,\beta}(x) = h_{\beta,\alpha}(-x)$ and

$$h_{\alpha,\beta}(x) = (n-\beta)\left[1+\frac{\alpha-\beta}{x^2}\left(1-\frac{3n-\alpha-2\beta}{x^2}\right)\right] + \mathcal{O}(x^{-6}) \tag{17}$$

as $x \to +\infty$ and the same expansion with α interchanged with β as $x \to -\infty$.

We have

Theorem 2. *The following holds for all real x and $n > 1/2$, except that the last inequality only holds for $n > 3/2$:*

$$\frac{1}{n+3/2}h_{\frac{1}{2},-\frac{3}{2}}(x) < \frac{1}{n+1/2}W_n(x) < 1 < \frac{1}{n-1/2}W_n(x) < \frac{1}{n-3/2}h_{\frac{3}{2},-\frac{1}{2}}(x).$$

Remark 6. The central inequalities $\frac{1}{n+1/2}W_n(x) < 1 < \frac{1}{n-1/2}W_n(x)$ reappeared in Ref. [7], but they were already proved in Ref. [8]. The first and last inequalities in this chain of inequalities were not correctly stated in Ref. [8, theorem 11]: the value $x = 0$ was erroneously set.

Remark 7. The first two inequalities in Theorem 2 (at the left) are sharp as $x \to +\infty$ while the two bounds at the right are sharp as $x \to -\infty$. The extreme bounds are sharper as two terms of the corresponding asymptotic expansions coincide, while for the central bounds only the dominant term is given. None of these bounds is simultaneously sharp as $x \to \pm\infty$, differently from the bounds we describe in the next section.

We notice that the function $W_n(x)$ has a sigmoidal shape similar to the functions $h_{\alpha,\beta}(x)$, $\alpha > \beta$ and that the selection $\alpha = 1/2$, $\beta = -1/2$ gives the exact limit values as $x \to \pm\infty$. We propose the following result valid for real x and $n > 1/2$ which we will be able to prove in Section 4:

$$W_n(x) > h_{\frac{1}{2},-\frac{1}{2}}(x). \tag{18}$$

Remark 8. The bound $h_{\frac{1}{2},-\frac{1}{2}}(x)$ is the best possible upper bound of the form $h_{\alpha,\beta}(x)$, because it is sharp both as $x \to \pm\infty$; in fact, the first two terms in the expansions are correct.

4 | BEYOND THE RICCATI BOUNDS

The previous analysis clearly suggests that $W_n(x)$ should be an increasing function of x. However, from the previous inequalities alone it does not seem possible to prove this result, which is known to be true and has been proved by indirect arguments.[7] Here, we give a direct proof of this result and, as a by-product of this analysis, we obtain the tightest available bounds for the ratios and double ratios of the PCFs. We expect that the same ideas can be applied to other monotonic special functions.

The idea is to construct a differential equation involving $W_n(x)$ and to analyze the nullclines, as done before. The analysis is not so straightforward as before, but it will be rewarding.

The starting point is the recurrence relation (3), which we multiply by $U(n-1,x)/U(n,x)^2$ yielding

$$(n+1/2)\frac{U(n+1,x)U(n-1,x)}{U(n,x)^2} + x\frac{U(n-1,x)}{U(n,x)} - \left(\frac{U(n-1,x)}{U(n,x)}\right)^2 = 0,$$

which in our notation is

$$W_n(x) = \Phi_n(x)(\Phi_n(x) - x). \tag{19}$$

We can simplify the Riccati equation (11) by substituting

$$\Phi_n(x) = \frac{x}{2} + \phi_n(x) \tag{20}$$

and we get:

$$\phi_n'(x) = \phi_n(x)^2 - V_n(x), \quad V_n(x) = \frac{x^2}{4} + n. \tag{21}$$

Now we have

$$W_n(x) = \phi_n(x)^2 - \frac{x^2}{4}, \tag{22}$$

and, because $\phi_n(x) > 0$ for all real x and $n > 1/2$ (Theorem 1),

$$\phi_n(x) = +\sqrt{\frac{x^2}{4} + W_n(x)}. \tag{23}$$

Taking the derivative of (22):

$$W_n'(x) = 2\phi_n(x)\phi_n'(x) - x/2 = 2\left(\phi_n(x)^3 - V_n(x)\phi_n(x) - \frac{x}{4}\right). \tag{24}$$

We can now substitute $\phi_n(x) = \sqrt{x^2/2 + W_n(x)}$ and we would have a differential equation relating $W_n'(x)$ with $W_n(x)$, and the analysis of the nullclines of the equation together with the asymptotic properties of the function $W_n(x)$ could be investigated to prove the monotonicity of the function and to obtain a bound. The analysis would be similar to the one considered before for $\Phi_n(x)$ in Section 3 with the difference that we do not have a Riccati equation now. It is however simpler to study the sign of (24) in terms of the values of $\phi_n(x)$ and to map the resulting results to the $x - W_n$ plane. For this idea, the first step is to solve for the values of $\phi_n(x)$ that make $W_n'(x) = 0$. The structure of these solutions is discussed next.

4.1 | Properties of the nullclines

In this subsection, we prove five lemmas in relation with Equation (24) and its nullclines that are needed for proving the main result of this paper (Theorem 3).

Lemma 2. *The cubic equation*

$$\lambda(x)^3 - V_n(x)\lambda_n(x) - \frac{x}{4} = 0 \tag{25}$$

has, for all real x and $n > 1/2$, three distinct real solutions.

Proof. We recall that given a cubic equation $ax^3 + bx^2 + cx + d = 0$, the equation has three different real solutions if the discriminant, given by

$$\Delta = 18abcd - 4b^3d + b^2c^2 - 4ac^3 - 27a^2d^2$$

is positive, while it has only one real solution (and two complex conjugate solutions) if $\Delta < 0$. Now with $a = 1$, $b = -V_n(x)$, and $c = -x/4$ we have

$$16\Delta(x) = 16\left\{-4(-V_n(x))^3 - 27\frac{x^2}{16}\right\} = x^6 + 12x^4n + (48n^2 - 27)x^2 + 64n^3. \tag{26}$$

That $\Delta(x) > 0$ for all real x is obvious for $|n| > 3/4$ because all the coefficients are positive in this case, but this is also true for all $|n| > 1/2$ as can be easily checked by computing the discriminant of the cubic equation $f(z) = 16\Delta(\sqrt{z}) = 0$. We have now $a = 1$, $b = 12n$, $c = 48n^2 - 27$, $d = 64$, and the discriminant of the third-degree polynomial $f(z)$ is $\tilde{\Delta} = 314928(-n^2 + \frac{1}{4})$, which is negative if $|n| > 1/2$, meaning that $f(z) = \Delta(\sqrt{z})$ has only one real root for z; such root must be negative, because on account of Descartes' rule of signs, $f(z)$ has exactly one negative real root if $|n| < 3/4$, which gives x purely imaginary. This proves that $\Delta(x)$ has no real roots if $|n| > 1/2$ and therefore $\Delta(x) > 0$ for all real x. ■

Lemma 3. *Denoting the three (real) solutions of (25) by $\lambda_n^-(x) < \lambda_n^0(x) < \lambda_n^+(x)$, we have, for all real x and $n > 1/2$, $\lambda_n^+(x) > 0$, $\lambda_n^-(x) = -\lambda_n^+(-x)$, and $\lambda_n^0(x) = -\lambda_n^0(-x)$, with sign$(\lambda_n^0(x))$ = sign$(-x)$.*

The positive solution can be written:

$$\lambda_n^+(x) = f_n(x)\cos\left(\frac{1}{3}\arccos\left(\frac{x}{f_n(x)^3}\right)\right), \quad f_n(x) = \sqrt{\frac{x^2 + 4n}{3}}.$$

Proof. We start giving an explicit expression for the roots using the well-known formula in terms of trigonometric functions, which is

$$\lambda(x) = \frac{2}{\sqrt{3}}\sqrt{V_n(x)}\cos\left(\frac{1}{3}\arccos\left(\frac{3\sqrt{3}x}{8V_n(x)^{3/2}}\right)+\psi\right), \tag{27}$$

with the three values $\psi = 0, \pm 2\pi/3$. Of course, the solutions are continuous and differentiable whenever the argument of the arc-cosine is smaller than 1 in absolute value, and this condition is equivalent to the positivity of the discriminant, which we have already proved for all real x and $n > 1/2$.

Now, because all the three roots are real and simple, and considering Descartes' rule of signs, we conclude that there is only one possible positive solution for $x > 0$, which is $\lambda_n^+(x)$, while the other two must be negative; similarly, for $x < 0$ there is only one negative solution and therefore two positive solutions.

Then $\lambda_n^+(x)$ must be positive for all real x. Now, because the cubic equation is invariant under the simultaneous changes $x \to -x$ and $\lambda(x) \to -\lambda(x)$, if $\lambda(x)$ solves the equation also does $-\lambda(-x)$. Therefore, $-\lambda_n^+(-x)$ is a second solution. And there is a third solution which must satisfy $\lambda(x) = -\lambda(-x)$, and therefore changes sign (and is zero at $x = 0$). Then we have $\lambda_n^0(x) = -\lambda_n^0(-x)$, while $\lambda_n^-(x) = -\lambda_n^+(-x)$. There is only one solution which is positive at $x = 0$, which is $\lambda_n^+(x)$, given by (27) with $\psi = 0$. ■

Lemma 4. *For all real x and $n > 1/2$, $\lambda_n^+(x)^2 > x^2/4$, $\lambda_n^-(x)^2 > x^2/4$, and $\lambda_n^0(x)^2 < x^2/4$.*

Proof. We make the substitution $\lambda(x) = \mu(x) - x/2$ in (25) and we have

$$2\mu(x)^3 - 3x\mu(x)^2 + (x^2 - 2n)\mu(x) + x(n - 1/2) = 0,$$

which for $x < 0$ has only one positive root, on account of Descartes' rule of signs; this solution has to be $\mu(x) = \lambda_n^+(x) + x/2$. Therefore, $\lambda_n^0(x) + x/2 < 0$ for $x < 0$ and, because $\lambda_n^0(x)$ is positive for $x < 0$, we have $|\lambda_n^0(x)| < |x|/2$ if $x < 0$; and since $\lambda_n^0(x) = -\lambda_n^0(-x)$ this inequality is true for all real x.

Finally, with the substitution $\lambda(x) = \mu(x) + x/2$ in (25) and with the same analysis using Descartes' rule of signs we conclude that $\lambda_n^+(x) - x/2 > 0$ for $x > 0$, which together with the previous condition for $x < 0$ ($\lambda_n^+(x) + x/2 > 0$) gives $\lambda_n^+(x) > |x|/2$. And because $\lambda_n^-(x) = -\lambda_n^+(-x)$ we also have that $\lambda_n^-(x) > |x|/2$. ■

There is only one additional lemma that we will need in the analysis of the nullclines for (24), namely:

Lemma 5. $w_n(x) = \lambda_n^+(x)^2 - \frac{x^2}{4}$ *is increasing as a function of x.*

Proof. We have

$$\omega_n'(x) = 2\lambda_n^+(x)\lambda_n^{+\prime}(x) - \frac{x}{2}. \tag{28}$$

Now differentiating

$$\lambda_n^+(x)^3 - V_n(x)\lambda_n^+(x) - \frac{x}{4} = 0, \tag{29}$$

we obtain

$$-\frac{x}{2}\lambda_n^+(x) - \frac{1}{4} + \lambda_n^{+\prime}(x)(3\lambda_n^+(x)^2 - V_n(x)) = 0$$

and then

$$\lambda_n^{+\prime}(x) = \frac{1 + 2x\lambda_n^+(x)}{4(3\lambda_n^+(x)^2 - V(x))}. \tag{30}$$

Now, inserting this in (28)

$$\omega_n'(x) = \frac{\lambda_n^+(x)(1 + 2x\lambda_n^+(x))}{2(3\lambda_n^+(x)^2 - V(x))} - \frac{x}{2} = \frac{1}{2}\frac{\lambda_n^+(x) + x(V(x) - \lambda_n^+(x)^2)}{3\lambda_n^+(x)^2 - V(x)},$$

and using (29) $V(x) - \lambda_n^+(x)^2 = -x/(4\lambda_n^+(x))$, and so

$$\omega_n'(x) = \frac{1}{2}\frac{\lambda_n^+(x)^2 - x^2/4}{\lambda_n^+(x)(3\lambda_n^+(x)^2 - V(x))}.$$

The numerator is positive because $\lambda_n^+(x)^2 - x^2/4 > 0$. With respect to the denominator

$$3\lambda_n^+(x)^2 - V(x) > \frac{3}{4}x^2 - \frac{x^2}{4} - n = \frac{x^2}{2} - n,$$

which is certainly positive for large enough $|x|$. A possible change of sign would be caused by a singularity in $\lambda_n^+(x)$ (see Equation 30) but this does not occur for $n > 1/2$, because $\lambda_n^+(x)$ is well defined and differentiable, as we saw. ■

From the study of the nullclines, and in particular of the only active nullcline for our problem, we can prove the next result, that will be used in establishing our main result.

Lemma 6. *Let $y(x)$ satisfy the differential equation*

$$y'(x) = 2\left(z(x)^3 - \left(\frac{x^2}{4} + n\right)z(x) - \frac{x}{4}\right), \quad n > 1/2, \tag{31}$$

where

$$z(x) = +\sqrt{\frac{x^2}{4} + y(x)}. \tag{32}$$

If $y(x)$ is positive and increasing as $x \to +\infty$ then

$$z(x) > \lambda_n^+(x) = f_n(x)\cos\left(\frac{1}{3}\arccos\left(\frac{x}{f_n(x)^3}\right)\right), \quad f_n(x) = \sqrt{\frac{x^2+4n}{3}},$$

$$y(x) > \lambda_n^+(x)^2 - \frac{x^2}{4}$$

and $y'(x) > 0$ for all real x.

Proof. Because $y(+\infty) > 0$ we have that $z(x) > x/2$ for large x. Then, denoting as before by $\lambda_n^-(x) < \lambda_n^0(x) < \lambda_+(x)$ the roots of $\lambda(x)^3 - (\frac{x^2}{4} + n)\lambda(x) - \frac{x}{4} = 0$, by Lemma 4 we have that $z(+\infty) > \lambda_n^0(x)$ because $z(x) > |x|/2$.

We are left with two possibilities, that $z(+\infty) > \lambda_n^+(+\infty)$ or the contrary, but because

$$y'(z) = 2(z(x) - \lambda_n^+(x))(z(x) - \lambda_n^0(x))(z(x) - \lambda_n^-(x))$$

and by hypotheses $y'(+\infty) > 0$ then necessarily $z(+\infty) > \lambda_n^+(+\infty)$.

However, this implies that $y(+\infty) = z(+\infty)^2 - \frac{x^2}{4} > w_n(+\infty)$ where $w_n(x) = \lambda_n^+(x)^2 - x^2/4$.

In other words, the function $y(x)$ lies above the curve $y = w_n(x)$, which is the active null-cline of the differential equation ($\lambda_n^0(x)$ and $\lambda_n^-(x)$ play no role because $z(x) = \sqrt{x^2/4 + y(x)} > |x|/2$). However, from Lemma 5 we know that $w_n'(x) > 0$, and therefore the fact that $y(+\infty) > w_n(+\infty)$ and that $y'(x) > 0$ for values of $y(x) > w_n(x)$ implies, by the same arguments used in Lemma 1, that $y(x) > w_n(x)$ for all real x and therefore that $y'(x) > 0$ for all x and, finally, $z(x) = \sqrt{x^2/4 + y(x)} > \sqrt{x^2/4 + w_n(x)} = \lambda_n^+(x)$. ∎

4.2 | Main results: Trigonometric and algebraic uniform lower bounds

We are now in the position to prove the main result of the paper, which provides very sharp bounds for the ratios and double ratios of the PCFs.

Theorem 3. *Let $\Phi_n(x) = \frac{U(n-1,x)}{U(n,x)}$ and $W_n(x) = (n+1/2)\frac{\Phi_n(x)}{\Phi_{n+1}(x)}$ then the following holds for all real x and $n > 1/2$:*

1. $\Phi_n(x) > 0$, $\Phi_n'(x) > 0$, $\Phi_n''(x) = W_n'(x) > 0$.
2. $\Phi_n(x) > \varphi_n(x) = \frac{x}{2} + \lambda_n^+(x)$.
3. $W_n(x) = (n-1/2) + \Phi_n'(x) > w_n(x) = \lambda_n^+(x)^2 - x^2/4$.

Proof. That $\Phi_n(x) > 0$, $\Phi_n'(x) > 0$ was proved in Theorem 1. The rest is a consequence of Lemma 6 because, on account of (10), we have that $W_n(+\infty) > 0$ and $W_n'(+\infty) > 0$. $W_n(x)$ plays the role of $y(x)$ in the lemma, and $\phi_n(x) = \Phi_n(x) - \frac{x}{2}$ plays the role of $z(x)$. ∎

Remark 9. The new bounds in Theorem 3 are sharp as $n \to +\infty$ (as all the bounds in this paper) and extremely sharp as $|x| \to +\infty$, particularly as $x \to +\infty$.

All the terms shown in (8) coincide with the expansion of the bound $\varphi_n(x)$ of the previous theorem, and we have that as $x \to +\infty$.

$$\frac{\Phi_n(x)}{\varphi_n(x)} - 1 = \frac{2n+1}{x^6} + \mathcal{O}(x^{-8}),$$

which is amazingly sharp, while as $x \to -\infty$

$$\frac{\Phi_n(x)}{\varphi_n(x)} - 1 = \frac{2}{x^4} + \mathcal{O}(x^{-6}),$$

which is not so sharp, but very sharp in any case.

Similarly, the bound for $W_n(x)$ is also very sharp as $x \to \pm\infty$ and we have that

$$w_n(x) = (n \pm 1/2)(1 - x^{-2}) + \left(\pm 3n^2 + 4n \pm \frac{5}{4}\right)x^{-4} + \mathcal{O}(x^{-6})$$

and then $W_n/w_n(x) - 1 = (2n \pm 1)x^{-4} + \mathcal{O}(x^{-6})$.

Next, we are proving that these lower bounds are tighter for all x than the upper bounds that were proved in the previous section, and even than the bound (18), which we will prove later.

Theorem 4. *The lower bound for $\Phi_n(x)$ of Theorem 3 is sharper than the bound of Theorem 1, that is:*

$$\lambda_n^+(x) > \frac{1}{2}\sqrt{x^2 + 4n - 2}, \quad n > 1/2, \quad x \in \mathbb{R}.$$

Proof. We prove that the bound (12) corresponds to a curve which lies below the nullcline $y = w_n(x)$ of (31), which in the $z(x)$ variable is $z = \lambda_n^+(x)$. To see this, we substitute $z(x)$ in (31) by the corresponding bound of $\phi_n(x) = \Phi_n(x) - x/2 = \sqrt{x^2 + 4n - 2}/2$ and we check that $y'(x) < 0$.

Indeed, setting $z(x) = \sqrt{x^2 + 4n - 2}/2$ in (24) we have

$$\frac{1}{2}y'(x) = -\frac{1}{2}z(x) - \frac{x}{4} < 0,$$

which completes the proof. ■

Next, we prove that the previously conjectured lower bound of (18) is smaller than $w_n(x)$, and therefore it is indeed a lower bound for $W_n(x)$.

Theorem 5. *For all real x and $n > 1/2$,*

$$W_n(x) > w_n(x) > w_n^{(a)}(x) = h_{\frac{1}{2},-\frac{1}{2}}(x),$$

and $w_n^{(a)}(x)$ is the best possible bound of the form $h_{\alpha,\beta}(x)$.

Proof. To see this, we check that if we take $y(x) = w_n^{(a)}(x)$ in (32) then we have $y'(x) < 0$ in (31), which means that the curve $y = w_n^{(a)}(x)$ lies below the nullcline $y = w_n(x)$, and therefore $w_n^{(a)}(x) < w_n(x)$; and because we have proved that $W_n(x) > w_n(x)$ then $W_n(x) > w_n(x) > w_n^{(a)}(x)$.

Indeed, taking $z(x) = h_{1/2,-1/2}(x)$ we have $y(x) = \sqrt{h_{\frac{1}{2},-\frac{1}{2}}(x) + \frac{x^2}{4}}$ and from this and using (31) we will have that $y'(x) < 0$ if

$$\sqrt{h_{\frac{1}{2},-\frac{1}{2}}(x) + x^2/4}\left(h_{\frac{1}{2},-\frac{1}{2}}(x) - n\right) - \frac{x}{4} < 0. \tag{33}$$

Now, we substitute $h_{\frac{1}{2},-\frac{1}{2}}(x)$ inside the square root by its supremum in $\mathbb{R}$, which is $(n + 1/2)$, and denoting

$$g_n(x) = \frac{1}{2}\sqrt{x^2 + 4n + 2}\left[(n + 1/2)\frac{x + \sqrt{x^2 + 4n - 2}}{x + \sqrt{x^2 + 4n + 2}} - n\right] - \frac{x}{4},$$

if we prove that $g_n(x) < 0$ then inequality (33) is proved. And after some elementary algebra

$$g_n(x) = -\frac{(n + 1/2)(x^2 + 4n - \sqrt{x^2 + 4n + 2}\sqrt{x^2 + 4n - 2})}{2(x + \sqrt{x^2 + 4n + 2})},$$

from where is it obvious that $g_n(x) < 0$ for all real x and $n > 1/2$. ■

Remark 10. The algebraic bound $w_n^{(a)}(x)$ is nearly as sharp as $w_n(x)$, because $w_n(x)/w_n^{(a)}(x) - 1 = (2n \pm 1)x^{-4} + \mathcal{O}(x^{-6})$.

Using the very sharp algebraic bound in Theorem 5 we can obtain easily a very sharp algebraic bound for $\Phi_n(x)$:

Corollary 3. *For all real x and $n > 1/2$, the following holds:*

$$\Phi_n(x) > \varphi_n^{(a)}(x) = \frac{x}{2} + \sqrt{\frac{x^2}{4} + w_n^{(a)}(x)} = \frac{x}{2} + \sqrt{\frac{x^2}{4} + \left(n + \frac{1}{2}\right)\frac{x + \sqrt{x^2 + 4n - 2}}{x + \sqrt{x^2 + 4n + 2}}}.$$

Remark 11. The bound of Corollary 3 has similar sharpness as the bound of Theorem 3 (but the relative difference with the value of $\Phi_n(x)$ is approximately two times bigger). Indeed, we have that as $x \to +\infty$

$$\frac{\Phi_n(x)}{\varphi_n^{(a)}(x)} - 1 = 2\frac{2n + 1}{x^6} + \mathcal{O}(x^{-8}),$$

while as $x \to -\infty$

$$\frac{\Phi_n(x)}{\varphi_n^{(a)}(x)} - 1 = \frac{4}{x^4} + \mathcal{O}(x^{-6}).$$

Corollary 4. *For $n > 1/2$ and $z > y$, we have:*

$$\frac{U(n,z)}{U(n,y)} < \exp\left(-\int_y^z \lambda_n^+(x)\,dx\right) \tag{34}$$

and

$$\frac{U(n,z)}{U(n,y)} < \exp\left(-\int_y^z \sqrt{\frac{x^2}{4} + w_n^{(a)}(x)}\,dx\right). \tag{35}$$

Proof. Using (2), we have that $\Phi_n(x) - \frac{x}{2} = -U'(n,x)/U(n,x)$. Therefore, from the bound of Corollary 3 we have

$$-\frac{U'(n,x)}{U(n,x)} > \sqrt{\frac{x^2}{4} + w_n^{(a)}(x)},$$

and the same can be written for the trigonometric bounds, changing $w_n^{(a)}(x)$ by $w_n(x) = \lambda_n^+(x)^2 - x^2/4$. Now the results follow after integration. ■

Remark 12. The bounds in Corollary 4 are given in terms of integrals of elementary functions, but the integrals cannot be expressed in terms of elementary functions. Still, explicit bounds in terms of elementary functions can be extracted by taking into account that $w_n(x)$ and $w_n^{(a)}(x)$ are increasing functions. Then, for instance, considering $z > y$ and using the trigonometric bound

$$\frac{U(n,z)}{U(n,y)} < \exp\left(-\int_y^z \sqrt{\frac{x^2}{4} + w_n(x)}\,dx\right) < \exp\left(-\int_y^z \sqrt{\frac{x^2}{4} + w_n(y)}\,dx\right).$$

And the last bound, though no so sharp, can be expressed in terms of elementary functions and is certainly sharper than the bound that can be extracted from Theorem 1, which is equivalent to replacing $w_n(y)$ with $w_n(-\infty) = n - 1/2$.

Using the known value of $U(n,0)$[15, 12.2.6] and taking $y = 0$, bounds for $U(n,z)$ are made available (which are not so sharp as the bounds for the ratios as $z \to \pm\infty$).

4.3 | Upper bounds

In the analysis, we have obtained very sharp lower bounds as $x \to \pm\infty$ for $\Phi_n(x)$, both of trigonometric ($\varphi_n(x)$, Theorem 3) and algebraic form ($\varphi_n^{(a)}(x)$, Corollary 3) and similarly very sharp bounds $w_n(x)$ (Theorem 3) and $w_n^{(a)}(x)$ (Theorem 5) for the double ratio $W_n(x)$, which drastically improve the bounds known so far. As done in Section 3, we can obtain upper bounds for $\Phi_n(x)$ from the lower bound by applying the recurrence relation both in the forward (16) and the backward (14) direction, and then from these upper bounds we can obtain also upper bounds for $W_n(x)$ using that $W_n(x) = \Phi_n(x) - x^2/4$.

We do not discuss these eight additional bounds in detail (for $\Phi_n(x)$ and $W_n(x)$ and starting from the bounds $\varphi_n(x)$ or $\varphi_n^{(a)}$ and with two different recursion directions), but only mention that the sharpness is preserved differently for the forward and the backward application of the recurrence (as also described in Section 3).

In the first place, we consider the bound from the backward recurrence, starting from $\varphi_n(x)$, and we have:

Corollary 5. *For all real x and $n > -1/2$, the following holds:*

$$\Phi_n(x) < \bar{\varphi}_n(x) = x + \frac{n+1/2}{\varphi_{n+1}(x)}.$$

As $x \to +\infty$

$$\frac{\Phi_n(x)}{\bar{\varphi}_n(x)} - 1 = \mathcal{O}(x^{-8}),$$

and as $x \to -\infty$

$$\frac{\Phi_n(x)}{\bar{\varphi}_n(x)} - 1 = \mathcal{O}(x^{-2}).$$

We conclude that $\bar{\varphi}_n(x)$ is sharper than $\varphi_n(x)$ as $x \to +\infty$ but less sharp for $x \to -\infty$. Differently from the backward recurrence, for the forward recurrence the sharpness as $x \to +\infty$ is maintained and improved as $x \to -\infty$, although the range of validity is restricted to $n > 3/2$:

Corollary 6. *For all real x and $n > 3/2$, the following holds:*

$$\Phi_n(x) < \tilde{\varphi}_n(x) = \frac{n-1/2}{-x+\varphi_{n-1}(x)}.$$

As $x \to +\infty$

$$\frac{\Phi_n(x)}{\tilde{\varphi}_n(x)} = \mathcal{O}(x^{-4}),$$

and as $x \to -\infty$

$$\frac{\Phi_n(x)}{\tilde{\varphi}_n(x)} - 1 = \mathcal{O}(x^{-8}).$$

Remark 13. Bounds for the ratio $U(n,y)/U(n,z)$ can also be established from the bounds in this section, similarly as done in Corollary 4. We skip the details for such bounds.

5 | NUMERICAL ILLUSTRATION OF THE SHARPNESS OF THE BOUNDS

To end the description of the new bounds, we estimate as a function of n the maximum errors for the bounds for all x in $\mathbb{R}$. This will give information on the global accuracy of the bounds. For this, we are estimating the errors as n becomes large using a simplification: we estimate that the maximum error takes place at $x = 0$. Let us recall that we are considering bounds which are very sharp as $x \to \pm\infty$. A more detailed analysis is possible using uniform asymptotics for the PCFs (see Ref. [15, 12.10.25]), but for our purpose it is enough with this simple analysis and we will see how this simplification is in fact quite reasonable for estimating these errors.

Because $W_n(0) = \Phi_n(0)^2$, the analysis for the errors for the bounds for $W_n(x)$ follow easily from those for $\Phi_n(0)$, and the relative accuracy of these bounds will be approximately twice the error for the bounds of $\Phi(x)$.

The values at $x = 0$ (see Ref. [15, 12.2.6]) are:

$$\Phi_n(0) = \sqrt{2}\frac{\Gamma\left(\frac{3}{4} + \frac{n}{4}\right)}{\Gamma\left(\frac{1}{4} + \frac{n}{2}\right)}$$

and

$$\varphi_n^{(0)}(0) = \sqrt{n - 1/2}, \quad \varphi_n(0) = \sqrt{n}, \quad \varphi_n^{(a)}(0) = (n^2 - 1/4)^{1/4},$$

where $\varphi_n^{(0)}(x)$ denotes the not so sharp bound of Theorem 1. Now, we estimate the relative accuracy as n becomes large by expanding in powers of n^{-1}.

We have

$$\begin{aligned}
\frac{\Phi_n(0)}{\varphi_n^{(0)}(0)} - 1 &= \frac{1}{4n} + \mathcal{O}(n^{-2}),\\
\frac{\Phi_n(0)}{\varphi_n(0)} - 1 &= \frac{1}{16n^2} + \mathcal{O}(n^{-4}).\\
\frac{\Phi_n(0)}{\varphi_n^{(a)}(0)} - 1 &= \frac{1}{8n^2} + \mathcal{O}(n^{-4}).
\end{aligned}$$

We observe that the new bounds are also sharper than the previous bounds $\varphi_n^{(0)}(x)$ as n becomes large, with a relative deviation decreasing quadratically. This means that, for instance, for $n > 10$ $\varphi_n(x)$ is an estimation for $\Phi_n(x)$ with at least two correct digits for all real x, and decreasing at least as $\mathcal{O}(x^{-4})$ as $|x|$ becomes large. As n becomes larger the situation of course improves and, for instance, for $n > 2500$ eight digits accuracy is attained for all real x. To our knowledge, such degree of uniformity and accuracy is without precedent in the estimation of nontrivial special functions depending on two parameters. The reason for this good behavior is the fact that the bounds are (very) sharp in three different directions: $x \to \pm\infty$ and $n \to +\infty$.

For the upper bounds $\bar{\varphi}_n(x)$ and $\tilde{\varphi}_n(x)$, the errors also decrease quadratically (they are roughly twice as large). Notice also that because we have upper and lower bounds which are similarly sharp as $x \to \pm\infty$ and $n \to +\infty$, it is possible to estimate the accuracy of the estimation by comparing the upper with the lower bound.

To illustrate this, we show in Figure 1 the plot of the curves

$$\epsilon = \frac{\tilde{\varphi}_n(x)}{\varphi_n(x)} - 1 \tag{36}$$

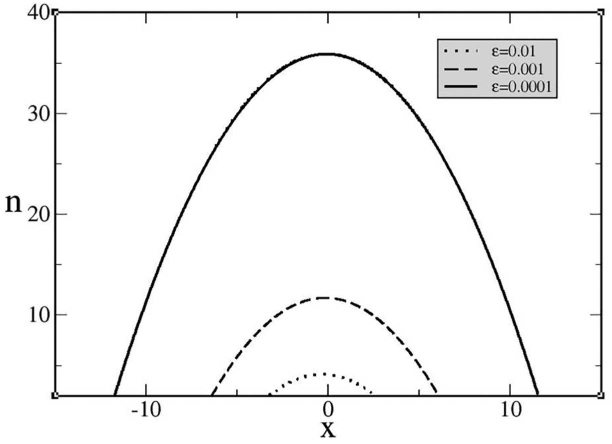

FIGURE 1 Curves $\epsilon = \frac{\tilde{\varphi}_n(x)}{\varphi_n(x)} - 1$ for three different values of ϵ

in the (x, n) plane and for three different values of ϵ which approximately correspond to three, four, and five correct digits. Notice that $\tilde{\varphi}_n(x)/\varphi_n(x) - 1 < \epsilon$ in the unbounded region outside the curve (36).

We conclude by commenting that bounding a function in terms of more elementary functions can be useful for extracting information from expressions which involve such functions without the need to compute them. This is maybe the most typical use of function bounds. However, in this case the bounds are so accurate that they can provide by themselves fairly accurate approximations for even moderate values of the variables. Because of the good accuracy of these bounds in unbounded domains in the (x, n)-plane, they will be useful in numerical algorithms for computing the PCFs. For instance, the bounds for $U(n-1, x)/U(n, x)$ can be used for estimating the tail of the continued fraction representation for this ratio when $x > 0$, accelerating in this way the convergence. A similar procedure was described in Ref. [12] for modified Bessel functions, and in the present case the new bounds are sharper and accurate in larger domains.

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DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no data sets were generated or analyzed during the current study.

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