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Bounding Standard Gaussian Tail Probabilities

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Abstract

We review various inequalities for Mills' ratio $(1 - \Phi)/\phi$, where ϕ and Φ denote the standard Gaussian density and distribution function, respectively. Elementary considerations involving finite continued fractions lead to a general approximation scheme which implies and refines several known bounds.

1 Introduction

Explicit formulae for the distribution function Φ of the standard Gaussian distribution are unknown, apart from various expansions, e.g. the series expansion

$$\Phi(x) = \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{2^k k! (2k+1)}$$

for real x, or the continued fractions expansion

for x > 0. Here $\phi = \Phi'$ denotes the standard Gaussian density. We refer to Abramowitz and Stegun (1972, Chapter 7) for these and numerous further results about the function Φ . The expansion (1) indicates that there should be good approximations or bounds on $1 - \Phi(x)$ of the form

$$1 - \Phi(x) \approx \frac{\phi(x)}{h(x)}, \quad x > 0,$$

with $h:(0,\infty)\to(0,\infty)$ being a relatively simple function. For instance, let $h_0(x):=x,\ h_1(x):=x+1/x$ and, for $k\geq 2$,

$$h_k(x) := x + \frac{1}{x + \frac{2}{\cdots x + \frac{k}{x}}}.$$

Then it is known that for integers $k \ge 0$ and arbitrary x > 0,

(2)
$$1 - \Phi(x) \begin{cases} < \\ > \end{cases} \frac{\phi(x)}{h_k(x)} \text{ if } k \text{ is } \begin{cases} \text{even,} \\ \text{odd.} \end{cases}$$

In particular,

$$\frac{\phi(x)}{x+1/x} < 1 - \Phi(x) < \frac{\phi(x)}{x},$$

which was first established by Gordon (1941). These special functions h_k and their properties have been investigated by numerous authors; we only refer to Shenton (1954), Pinelis (2002), Baricz (2008) and the references therein.

While the previous bounds are only useful for x bounded away from zero, some authors provided inequalities on the whole interval $[0, \infty)$ or even larger sets. Indeed, Komatu (1955) showed that

(3)
$$\frac{2\phi(x)}{\sqrt{4+x^2+x}} < 1 - \Phi(x) < \frac{2\phi(x)}{\sqrt{2+x^2+x}} \quad \text{for } x \ge 0;$$

see also Ito and McKean (1974). In fact, the lower bound is due to Birnbaum (1942) who formulated it equivalently as

$$\frac{\sqrt{4+x^2}-x}{2}\phi(x) < 1-\Phi(x) \text{ for } x \ge 0.$$

Pollak (1956) refined Komatu's upper bound as follows:

(4)
$$1 - \Phi(x) < \frac{2\phi(x)}{\sqrt{8/\pi + x^2} + x} \quad \text{for } x > 0.$$

An alternative upper bound, due to Sampford (1953) and rediscovered by Szarek and Werner (1999), reads

(5)
$$1 - \Phi(x) < \frac{4\phi(x)}{\sqrt{8 + x^2 + 3x}} \quad \text{for } x \ge 0.$$

Shenton (1954) and Kouba (2006) generalized Komatu's bound (3) and Sampford's bound (5) substantially. Here is a reformulation of their bounds with continued fractions: For integers $k \geq 0$ and j = 1, 2 define $h_{k,j} : [0, \infty) \to (0, \infty)$ via

$$h_{0,j}(x) := \sqrt{j/2 + (x/2)^2} + x/2, \quad h_{1,j}(x) := x + \frac{1}{\sqrt{1 + j/2 + (x/2)^2} + x/2},$$

and, if $k \geq 2$,

$$h_{k,j}(x) = x + \frac{1}{x + \frac{2}{x + \frac{k}{\sqrt{k + j/2 + (x/2)^2} + x/2}}}$$

Then for all $x \geq 0$ and integers $m \geq 0$,

(6)
$$\frac{\phi(x)}{h_{2m,2}(x)} < 1 - \Phi(x) < \frac{\phi(x)}{h_{2m,1}(x)},$$

(7)
$$\frac{\phi(x)}{h_{2m+1,1}(x)} < 1 - \Phi(x) < \frac{\phi(x)}{h_{2m+1,2}(x)}.$$

In the present manuscript we present all these bounds in a common framework and propose refinements. In Section 2 we consider the derivative of $\phi/h - (1-\Phi)$ for a smooth function $h:(0,\infty)\to(0,\infty)$ with $\lim_{x\to\infty}h(x)=\infty$, and these elementary considerations yield the bounds (3), (4), (5) and a new lower bound. In Section 3 we consider approximations ϕ/h_k of $1-\Phi$, where

$$h_k(x) = x + \frac{1}{x + \frac{2}{x + \frac{k-1}{x + \frac{k}{g_k(x)}}}}$$

with smooth functions $g_k:(0,\infty)\to(0,\infty)$. It turns out that under general conditions on g_k , this yields upper and lower bounds ϕ/h_k of $1-\Phi$.

In Section 4, we consider functions $g_k(x)$ of the form

$$q_k(x) = \sqrt{c_k + (x/2)^2} + x/2$$

with special constants $c_k \in [k+1/2, k+1]$, and this improves the bounds (6) and (7). In Section 5 we consider

$$g_k(x) = \sqrt{c_k} + \lambda_k x$$

with an additional constant $\lambda_k > 0$, which leads to purely rational functions h_k . The resulting bounds are compared to those in Section 4. These rational functions h_k may be improved substantially be considering

$$g_k(x) = \sqrt{c_k} \exp(-\delta_k x) + x$$

for some $\delta_k > 0$ as explained in Section 6.

Finally, in Section 7 we describe briefly a recurrence scheme to represent the functions h_k as ratios p_k/q_k rather than continued fractions.

2 First Steps

Let $h:(0,\infty)\to(0,\infty)$ be a differentiable function with $\lim_{x\to\infty}h(x)=\infty$. Then the approximation error

$$\Delta(x) := \frac{\phi(x)}{h(x)} - (1 - \Phi(x))$$

satisfies

$$\lim_{x \to \infty} \Delta(x) = 0$$

and

(9)
$$\Delta'(x) = \frac{\phi(x)}{h(x)^2} (h(x)^2 - xh(x) - h'(x)).$$

Consider first h(x) = x. Then $h(x)^2 - xh(x) - h'(x) = -1$, so $\Delta' < 0$ on $(0, \infty)$. Together with (8) we obtain that $\Delta > 0$, which is inequality (2) for k = 0. However, in view of the bounds (3) and (4) of Komatu and Pollak, we try

$$h(x) := \sqrt{c + (x/2)^2} + x/2 = \frac{\sqrt{4c + x^2} + x}{2}$$

for some c > 0 to be specified later. Then Δ is well defined and continuous on $[0, \infty)$, and one verifies easily that

$$h(x)^2 - xh(x) - h'(x) = c - 1/2 - t(x,c)/2$$

where

$$t(x,c) := \frac{x}{\sqrt{4c+x^2}}.$$

Note that $t(\cdot,c):[0,\infty)\to[0,1)$ is bijective and increasing. In case of c=1,

$$\operatorname{sign}(\Delta'(x)) = \operatorname{sign}(1 - t(x, c)) = +1.$$

Thus $\Delta < 0$ on $[0, \infty)$, and we rediscover Komatu's lower bound in (3). Setting c = 1/2, we realize that

$$\operatorname{sign}(\Delta'(x)) = \operatorname{sign}(-t(x,c)) = -1,$$

so $\Delta > 0$ on $[0, \infty)$, which implies the upper bound in (3).

Note that

$$\Delta(0) = 0$$
 if, and only if, $h(0) = \sqrt{2/\pi}$.

The latter condition is satisfied if $c = 2/\pi$, which corresponds to Pollak's function

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

Indeed,

$$\operatorname{sign}(\Delta'(x)) = \operatorname{sign}(2c - 1 - t(x, c)) = \operatorname{sign}\left(\frac{4 - \pi}{\pi} - t(x, 2/\pi)\right).$$

Thus $\Delta' > 0$ on $(0, x_o)$ and $\Delta' < 0$ on (x_o, ∞) , where x_o solves the equation $t(x_o, 2/\pi) = (4 - \pi)/\pi \in (0, 1)$. This shows that $\Delta > 0$ on $(0, \infty)$, and we obtain Pollak's upper bound (4).

Now we go one step further: Since

$$\frac{\sqrt{4c+x^2}+x}{2} = x + \frac{\sqrt{4c+x^2}-x}{2} = x + \frac{2c}{\sqrt{4c+x^2}+x},$$

we consider functions h of the form

$$h(x) = x + \frac{1}{g(x)}$$

with $g:(0,\infty)\to(0,\infty)$ differentiable. One can easily verify that

$$h(x)^2 - xh(x) - h'(x) = -\frac{g(x)^2 - xg(x) - 1 - g'(x)}{g(x)^2},$$

so

$$\operatorname{sign}(\Delta'(x)) = \operatorname{sign}(h(x)^2 - xh(x) - h'(x))$$
$$= -\operatorname{sign}(g(x)^2 - xg(x) - 1 - g'(x)).$$

In case of g(x) = x, we obtain $sign(\Delta'(x)) = +1$, so $\Delta > 0$ on $(0, \infty)$, i.e. (2) holds for k = 1. Again we can refine this considerably by considering

$$g(x) = \sqrt{c + (x/2)^2} + x/2$$

for some c > 0. This leads to

$$h(x) = x + \frac{2}{\sqrt{4c + x^2} + x} = x + \frac{\sqrt{4c + x^2} - x}{2c}$$
$$= \frac{(2c - 1)x + \sqrt{4c + x^2}}{2c},$$

and

$$sign(\Delta'(x)) = -sign(c - 1 - g'(x)) = -sign(2c - 3 - t(x, c)).$$

For c=2, the latter sign equals -1 for all x>0, so $\Delta>0$ on $[0,\infty)$, and we obtain the upper bound (5) of Sampford. On the other hand, if $c=\pi/2$, then $h(0)=1/g(0)=\sqrt{2/\pi}$, so $\Delta(0)=0$, and

$$\operatorname{sign}(\Delta'(x)) = -\operatorname{sign}(\pi - 3 - t(x, \pi/2)).$$

Thus $\Delta' < 0$ on $(0, x_o)$ and $\Delta' > 0$ on (x_o, ∞) , where $t(x_o, \pi/2) = \pi - 3 \in (0, 1)$, and we obtain a new lower bound:

(10)
$$1 - \Phi(x) > \frac{\pi \phi(x)}{(\pi - 1)x + \sqrt{2\pi + x^2}} \quad \text{for } x > 0.$$

This corresponds to

$$h(x) = x + \frac{2}{\sqrt{2\pi + x^2} + x}$$

which is strictly smaller than the function

$$h(x) = x + \frac{2}{\sqrt{4 + x^2} + x}$$

corresponding to Komatu's lower bound in (3).

Figure 1 illustrates the bounds we have seen so far. Precisely, it shows the approximation error $\Delta = \phi/h - (1 - \Phi)$ for Komatu's lower bound (3), the new lower bound (10) as well as the upper bounds (4) of Pollak and (5) of Sampford.

3 Continued Fractions and General Bounds

Recall that we started with an arbitrary function h(x), then turned our attention to h(x) = x + 1/g(x) with smooth g, and the special functions g we used may also be written as $g(x) = x + 1/\tilde{g}(x)$ with another smooth function $\tilde{g} > 0$. After playing around with the resulting approximation error $\Delta = \phi/h - (1 - \Phi)$ and $\operatorname{sign}(\Delta')$, the following scheme seems to be promising:

$$h(x) = g_0(x) = x + \frac{1}{g_1(x)} = x + \frac{1}{x + \frac{2}{g_2(x)}}$$

for some differentiable function $g_2:(0,\infty)\to(0,\infty)$. Indeed, elementary calculations reveal that

$$sign(\Delta'(x)) = sign(g_0(x)^2 - xh_0(x) - 0 - g'_0(x))$$

$$= -sign(g_1(x)^2 - xg_1(x) - 1 - g'_1(x))$$

$$= sign(g_2(x)^2 - xg_2(x) - 2 - g'_2(x)),$$

and this suggests a more general result which will be proved via induction:

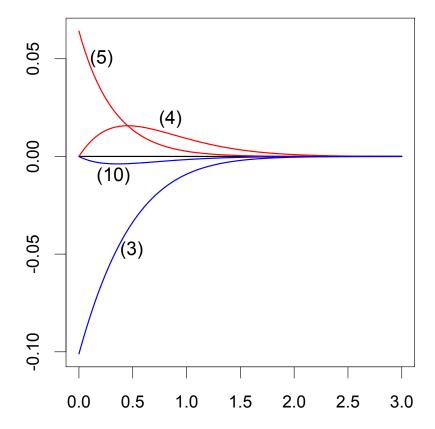


Figure 1: Approximation errors Δ after first steps.

Lemma 1. Let $g_0, g_1, g_2, ...$ be differentiable functions from $(0, \infty)$ to $(0, \infty)$, and define

$$h_0(x) := g_0(x), \quad h_1(x) := x + \frac{1}{g_1(x)}, \quad h_2(x) := x + \frac{1}{x + \frac{2}{g_2(x)}}$$

and, for integers k > 2,

$$h_k(x) := x + \frac{1}{x + \frac{2}{x + \frac{k-1}{x + \frac{k}{q_k(x)}}}}.$$

Then the approximation errors $\Delta_k := \phi/h_k - (1 - \Phi)$ satisfy

$$\operatorname{sign}(\Delta'_k(x)) = (-1)^k \operatorname{sign}(g_k(x)^2 - xg_k(x) - k - g'_k(x)).$$

Proof of Lemma 1. We know that the claim is correct for k = 0, 1. Now suppose that it is correct for an arbitrary integer $k \ge 1$, and let $g_k(x) = x + (k+1)/g_{k+1}(x)$

for a differentiable function $g_{k+1}:(0,\infty)\to(0,\infty)$. Then

$$g_{k}(x)^{2} - xg_{k}(x) - k - g'_{k}(x)$$

$$= g_{k}(x)(g_{k}(x) - x) - k - g'_{k}(x)$$

$$= \left(x + \frac{k+1}{g_{k+1}(x)}\right) \frac{k+1}{g_{k+1}(x)} - k - 1 + \frac{(k+1)g'_{k+1}(x)}{g_{k+1}(x)^{2}}$$

$$= -\frac{k+1}{g_{k+1}(x)^{2}} \left(g_{k+1}(x)^{2} - xg_{k+1}(x) - (k+1) - g'_{k+1}(x)\right).$$

In particular, sign $(\Delta'(x))$ equals

$$(-1)^{k+1}\operatorname{sign}\Big(g_{k+1}(x)^2 - xg_{k+1}(x) - (k+1) - g'_{k+1}(x)\Big).$$

With Lemma 1 at hand we can derive bounds for $1-\Phi$, similarly as in Section 2. Note first that $g_k(x) := x$ yields $g_k(x)^2 - xg_k(x) - k - g'_k(x) = -(k+1)$, so the corresponding approximation error Δ satisfies $\operatorname{sign}(\Delta'(x)) = (-1)^{k+1}$. This implies (2) for arbitrary $k \geq 1$. But Lemma 1 leads to a refined criterion:

Lemma 2. In the setting of Lemma 1, suppose that g_k is defined and continuous on $[0, \infty)$ such that $h_k(0) = \sqrt{2/\pi}$, i.e. $\Delta_k(0) = 0$. If there exists a point $x_k > 0$ such that

$$sign(g_k(x)^2 - xg_k(x) - k - g'_k(x)) = sign(x_k - x),$$

then $\Delta_k > 0$ on $(0, \infty)$ for even k, and $\Delta_k < 0$ on $(0, \infty)$ for odd k.

The requirement that $h_k(0) = \sqrt{2/\pi}$ for k = 0, 1, 2, ... means that $c_k^* := g_k(0)^2$ satisfies

(11)
$$c_0^* = \frac{2}{\pi} \text{ and } c_k^* = \frac{k^2}{c_{k-1}^*} \text{ for } k = 1, 2, 3, \dots$$

In other words,

(12)
$$c_0^* = \frac{2}{\pi}$$
, $c_1^* = \frac{\pi}{2}$ and $c_k^* = \left(\frac{k}{k-1}\right)^2 c_{k-2}^*$ for $k = 2, 3, 4, \dots$

This leads to

(13)
$$c_{2m}^* = \left(\frac{2 \cdot 4 \cdot 6 \cdots (2m)}{1 \cdot 3 \cdot 5 \cdots (2m-1)}\right)^2 \frac{2}{\pi},$$

(14)
$$c_{2m+1}^* = \left(\frac{1 \cdot 3 \cdot 5 \cdot \cdots (2m+1)}{2 \cdot 4 \cdot \cdots (2m)}\right)^2 \frac{\pi}{2}$$

for integers $m \geq 1$. For later purposes it is crucial to have good bounds for these constants c_k^* . Numerical experiments led to the formulation of the following result:

Lemma 3. The constants c_k^* just introduced satisfy

$$\frac{1}{8(k+1)} < c_k^* - k - 1/2 < \frac{1}{8c_k^*} < \frac{1}{8(k+1/2)}$$
 for all $k \ge 0$.

The proof of this lemma will be postponed to the next section, because there we get the initial bound $k + 1/2 < c_k^* < k + 1$ almost for free.

Remark 1. Note that for even integers $k \geq 2$,

$$\sqrt{c_k^*} = \sqrt{2/\pi} \, 2^k \binom{k}{k/2}^{-1},$$

so Lemma 3 yields

$$\sqrt{\pi} \binom{k}{k/2} 2^{-(k+1/2)} \sqrt{k+1/2} = \sqrt{\frac{k+1/2}{c_k^*}} \in \left[1 - \frac{1}{16(k+1/2)^2}, 1\right].$$

4 Refining Shenton's Bounds

Starting from Lemma 1 we consider

$$q_k(x) := \sqrt{c_k + (x/2)^2} + x/2 > x$$

for some constant $c_k > 0$ yet to be specified. Now

$$g_k(x)^2 - xg_k(x) - k - g'_k(x) = c_k - k - 1/2 - t(x, c_k)/2.$$

Thus

$$\operatorname{sign}(\Delta'_k(x)) = (-1)^k \operatorname{sign}(2(c_k - k - 1/2) - t(x, c_k)).$$

In case of $c_k = k + 1$, the right hand side equals $(-1)^k \operatorname{sign}(1 - t(x, c_k)) = (-1)^k$, and for $c_k = k + 1/2$, the right hand side equals $(-1)^k \operatorname{sign}(-t(x, c_k)) = (-1)^{k+1}$ for all x > 0. This leads to Shenton's and Kouba's strikt bounds in (6) and (7). It entails also that the constants c_k^* from the previous section satisfy

$$c_k^* \in (k+1/2, k+1).$$

For $h_k(0)$ is a continuous and strictly monotone function of $c_k \in [k+1/2, k+1]$ with extremal values being strictly smaller and strictly larger than $\sqrt{2/\pi}$. Setting $c_k = c_k^*$ yields a function g_k satisfying the criterion of Lemma 2 with x_k solving the equation

$$t(x_k, c_k^*) = 2(c_k^* - k - 1/2) \in (0, 1),$$

i.e.

(15)
$$x_k = \frac{2\sqrt{c_k^*}(c_k^* - k - 1/2)}{\sqrt{1/4 - (c_k^* - k - 1/2)^2}} = \frac{2\sqrt{c_k^*}(c_k^* - k - 1/2)}{\sqrt{(c_k^* - k)(k + 1 - c_k^*)}}$$

These considerations yield already the first part of our main result.

Theorem 1. Let

$$h_0(x) := \sqrt{2/\pi + (x/2)^2} + x/2, \quad h_1(x) := x + \frac{1}{\sqrt{\pi/2 + (x/2)^2} + x/2}$$

and, for integers $k \geq 2$,

$$h_k(x) := x + \frac{1}{x + \frac{2}{\cdots x + \frac{k}{\sqrt{c_k^* + (x/2)^2} + x/2}}}.$$

Then the approximation errors $\Delta_k := \phi/h_k - (1-\Phi)$ satisfy the following inequalities:

$$\Delta_0 > \Delta_2 > \Delta_4 > \cdots > 0$$
 and $\Delta_1 < \Delta_3 < \Delta_5 < \cdots < 0$

on $(0, \infty)$. Moreover,

$$\max_{x>0} |\Delta_k(x)| = |\Delta_k(x_k)| < \frac{1}{32(k+1/2)^2}$$

with x_k given by (15).

Remark 2. The first three bounds ϕ/h_k from Theorem 1 are given by the following functions h_k :

$$h_0(x) = \frac{\sqrt{8/\pi + x^2} + x}{2},$$

$$h_1(x) = x + \frac{1}{\sqrt{\pi/2 + (x/2)^2} + x/2} = \frac{(\pi - 1)x + \sqrt{2\pi + x^2}}{\pi},$$

$$h_2(x) = x + \frac{1}{x + \frac{2}{\sqrt{8/\pi + (x/2)^2} + x/2}} = x + \frac{8/\pi}{(8/\pi - 1)x + \sqrt{32/\pi + x^2}}.$$

Note that the upper bound ϕ/h_2 for $1-\Phi$ is better than Pollak's upper bound ϕ/h_0 in (4). It is also better than the upper bound (5) of Sampford, because the latter equals ϕ/h with

$$h(x) = x + \frac{1}{\sqrt{2 + (x/2)^2} + x/2} = x + \frac{1}{x + \frac{2}{\sqrt{2 + (x/2)^2} + x/2}} < h_2(x)$$

for x > 0.

Figure 2 shows the approximation errors Δ_k from Theorem 1 for some choices of k. On the left hand side one sees $\Delta_0, \Delta_1, \ldots, \Delta_5$. Note that the worst functions Δ_0, Δ_1 correspond to the bounds (4) and (10), respectively, also depicted in Figure 1. On the right hand side one sees $\Delta_2, \Delta_3, \ldots, \Delta_9$.

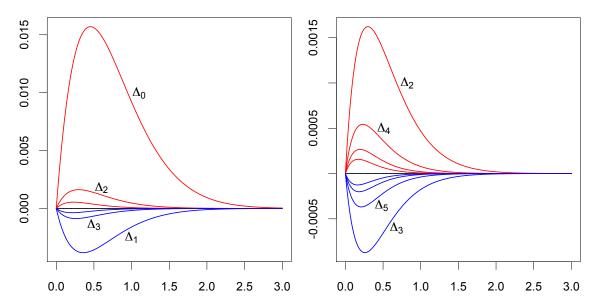


Figure 2: Approximation errors Δ_k for k = 0, 1, ..., 5 (left) and k = 2, 3, ..., 9 (right).

Before proving Theorem 1 we have to prove Lemma 3:

Proof of Lemma 3. As we have just shown, $k+1/2 < c_k^* < k+1$. Now we compare c_k^* with $d_k := k+1/2 + \left(8(k+\gamma)\right)^{-1}$ for some fixed $\gamma > 0$. Note that

$$\lim_{k \to \infty} \frac{c_k^*}{k} = \lim_{k \to \infty} \frac{d_k}{k} = 1.$$

Suppose we can show that

(17)
$$\frac{c_k^*}{d_k} < \frac{c_{k+2}^*}{d_{k+2}} for all k \ge 0.$$

Then, for arbitrary integers $k \geq 0$, the sequence $(c_{k+2\ell}/d_{k+2\ell})_{\ell=0}^{\infty}$ is strictly increasing with limit

$$\lim_{\ell \to \infty} \frac{c_{k+2\ell}^*}{d_{k+2\ell}} = \lim_{\ell \to \infty} \frac{c_{k+2\ell}^*/(k+2\ell)}{d_{k+2\ell}/(k+2\ell)} = 1,$$

whence $c_k^* < d_k$. Analogously, if

(18)
$$\frac{c_k^*}{d_k} > \frac{c_{k+2}^*}{d_{k+2}} \text{ for all } k \ge 0,$$

then $c_k^* > d_k$ for each $k \ge 0$.

Writing $x \sim y$ if $x = \tau y$ with $\tau > 0$, we may deduce from (12) that

$$\frac{c_{k+2}^*}{d_{k+2}} - \frac{c_k^*}{d_k} \sim (k+2)^2 d_k - (k+1)^2 d_{k+2}
= (k+2)^2 d_k - (k+1)^2 d_{k+2}
= (k+2)^2 (k+1/2) - (k+1)^2 (k+5/2) + \frac{(k+2)^2}{8(k+\gamma)} - \frac{(k+1)^2}{8(k+2+\gamma)}
= -\frac{1}{2} + \frac{(k+2)^2}{8(k+\gamma)} - \frac{(k+1)^2}{8(k+2+\gamma)}
\sim (k+2)^2 (k+2+\gamma) - 4(k+\gamma)(k+2+\gamma) - (k+1)^2 (k+\gamma)
= (3-6\gamma)k + 8 - 5\gamma - 4\gamma^2.$$

In case of $\gamma = 1/2$, the previous expression equals 9/2, so (17) is satisfied. In case of $\gamma = 1$ we get -3k - 1, so (18) holds true.

It remains to prove the refined upper bound $c_k^* \leq d_k := k + 1/2 + (8c_k^*)^{-1}$ for arbitrary $k \geq 0$. Since the latter constants satisfy (16), too, it suffices to verify (17). Tedious but elementary manipulations show that this is now equivalent to

$$c_k < k + 1/2 + \frac{k + 7/4}{(k+2)^2},$$

and the right hand side is easily shown to be larger than our preliminary bound $k+1/2+\left(8(k+1/2)\right)^{-1}$ for c_k^* .

Proof of Theorem 1. Our previous considerations show already that $1-\Phi < \phi/h_k$ for even k and $1-\Phi > \phi/h_k$ for odd k on $(0,\infty)$. To verify that $\phi/h_0 > \phi/h_2 > \phi/h_4 > \cdots$ and $\phi/h_1 < \phi/h_3 < \phi/h_5 < \cdots$, it suffices to show that for any integer $k \ge 0$ and x > 0,

$$\sqrt{c_k^* + (x/2)^2} + x/2 = x + \frac{c_k^*}{\sqrt{c_k^* + (x/2)^2} + x/2}$$

is strictly smaller than

(19)
$$x + \frac{k+1}{x + \frac{k+2}{\sqrt{c_{k+2}^* + (x/2)^2} + x/2}}.$$

To this end, recall that $c_{k+2}^* = c_k^*/\rho_k^2$ with $\rho_k := (k+1)/(k+2) \in [1/2,1)$ by (12).

Consequently, (19) equals

$$x + \frac{k+1}{x + \frac{k+1}{\sqrt{c_k^* + (\rho_k x/2)^2} + \rho_k x/2}}$$

$$= x + \frac{(k+1)c_k^*}{c_k^* x + (k+1)\left(\sqrt{c_k^* + (\rho_k x/2)^2} - \rho_k x/2\right)}$$

$$= x + \frac{c_k^*}{\sqrt{c_k^* + (\rho_k x/2)^2} + (2c_k^*/(k+1) - \rho_k)x/2}$$

Hence we have to show that

$$\sqrt{c_k^* + (\rho_k x/2)^2} + (2c_k^*/(k+1) - \rho_k)x/2 < \sqrt{c_k^* + (x/2)^2} + x/2,$$

that means.

$$(2c_k^*/(k+1) - \rho_k - 1)x/2 < \sqrt{c_k^* + (x/2)^2} - \sqrt{c_k^* + (\rho_k x/2)^2}$$

$$= \frac{(1 - \rho_k^2)(x/2)^2}{\sqrt{c_k^* + (x/2)^2} + \sqrt{c_k^* + (\rho_k x/2)^2}}.$$

Dividing both sides by x/2, one realizes that the previous inequality holds for all x > 0 if, and only if, $2c_k^*/(k+1) - \rho_k - 1 \le 0$, which is equivalent to

$$c_k^* \le \frac{(k+1)(k+3/2)}{k+2} = k+1/2 + \frac{1}{2k+4}.$$

But this inequality is weaker than and thus a consequence of the upper bound in Lemma 3.

Let $\tilde{\Delta}_k := \phi/\tilde{h}_k - (1-\Phi)$, where \tilde{h}_k is defined as h_k with k+1/2 in place of c_k^* , so $\operatorname{sign}(\tilde{\Delta}_k') = (-1)^{k+1}$. Thus $0 \le \Delta_k < \tilde{\Delta}_k$ with $\tilde{\Delta}_k$ strictly decreasing, if k is even, while $0 \ge \Delta_k > \tilde{\Delta}_k$ with $\tilde{\Delta}_k$ strictly increasing, if k is odd. In case of even k, $\max_{x \ge 0} \Delta_k(x)$ is strictly smaller than

$$\tilde{\Delta}_k(0) = \tilde{\Delta}_k(0) - \Delta_k(0) = \frac{\phi(0)}{h_k(0)} \left(\frac{h_k(0)}{\tilde{h}_k(0)} - 1 \right) = \frac{1}{2} \left(\sqrt{\frac{c_k^*}{k + 1/2}} - 1 \right)$$

while in case of odd k, $\max_{x\geq 0} |\Delta_k(x)|$ is strictly smaller than

$$-\tilde{\Delta}_{k}(0) = \Delta_{k}(0) - \tilde{\Delta}_{k}(0) = \frac{\phi(0)}{h_{k}(0)} \left(1 - \frac{\tilde{h}_{k}(0)}{h_{k}(0)}\right) = \frac{1}{2} \left(1 - \sqrt{\frac{k+1/2}{c_{k}^{*}}}\right)$$

$$< \frac{1}{2} \left(\sqrt{\frac{c_{k}^{*}}{k+1/2}} - 1\right).$$

Since $c_k^* \le k + 1/2 + (8(k+1/2))^{-1} = (k+1/2)(1 + (8(k+1/2)^2)^{-1})$ by Lemma 3,

$$\frac{1}{2} \left(\sqrt{\frac{c_k^*}{k+1/2}} - 1 \right) < \frac{1}{4} \left(\frac{c_k^*}{k+1/2} - 1 \right) \le \frac{1}{32(k+1/2)^2}.$$

5 Rational Bounds

It is also possible to obtain approximations ϕ/\widetilde{h}_k of $1-\Phi$ with rational functions $\widetilde{h}_k:[0,\infty)\to(0,\infty)$. To this end, consider h_k as in Lemma 1 with the simpler function

$$g_k(x) := \sqrt{c_k^*} + \lambda_k x$$

for some $\lambda_k \in [0,1]$ yet to be specified. Now

$$g_k(x)^2 - xg_k(x) - k - g'_k(x) = \sqrt{c_k^*} (2\lambda_k - 1)x - \lambda_k (1 - \lambda_k)x^2 + c_k^* - k - \lambda_k.$$

Suppose first that $\lambda_k = 1$. Then the previous display equals $\sqrt{c_k^*} x - (k+1-c_k^*)$, so

$$\operatorname{sign}(\Delta'_k(x)) = (-1)^k \operatorname{sign}\left(x - \frac{k+1-c_k^*}{\sqrt{c_k^*}}\right).$$

Hence for even k, ϕ/h_k is a lower bound $1 - \Phi$, whereas for odd k it is an upper bound. Numerical experiments showed, however, that the bounds in Section 4 are better.

More interesting is the choice $\lambda_k := c_k^* - k \in (1/2, 1)$. Then

$$g_k(x)^2 - xg_k(x) - k - g'_k(x) = x(a_k - b_k x)$$

with $a_k := 2\sqrt{c_k^*}(c_k^* - k - 1/2)$ and $b_k := (c_k^* - k)(k + 1 - c_k^*)$. Thus g_k satisfies the criterion in Lemma 2 with x_k equal to

(20)
$$\widetilde{x}_k := \frac{2\sqrt{c_k^*(c_k^* - k - 1/2)}}{(c_k^* - k)(k + 1 - c_k^*)} = \frac{2\sqrt{c_k^*(c_k^* - k - 1/2)}}{1/4 - (c_k^* - k - 1/2)^2}.$$

These considerations yield already the first part of our second main result:

Theorem 2. Let

$$\widetilde{h}_0(x) := \sqrt{2/\pi} + (2/\pi)x, \quad \widetilde{h}_1(x) := x + \frac{1}{\sqrt{\pi/2} + (\pi/2 - 1)x}$$

and, for integers $k \geq 2$,

$$\widetilde{h}_k(x) := x + \frac{1}{x + \frac{2}{\cdots x + \frac{k}{\sqrt{c_k^* + (c_k^* - k)x}}}}.$$

Then the approximation errors $\widetilde{\Delta}_k := \phi/\widetilde{h}_k - (1-\Phi)$ satisfy the following inequalities:

$$\widetilde{\Delta}_0 \ > \ \widetilde{\Delta}_2 \ > \ \widetilde{\Delta}_4 \ > \ \cdots \ > \ 0 \quad \text{and} \quad \widetilde{\Delta}_1 \ < \ \widetilde{\Delta}_3 \ < \ \widetilde{\Delta}_5 \ < \ \cdots \ < \ 0$$

on $(0, \infty)$. Moreover, the approximation errors $\widetilde{\Delta}_k$ and Δ_k (as in Theorem 1) satisfy the following inequalities:

$$\max_{x>0} \left| \widetilde{\Delta}_k(x) \right| = \left| \widetilde{\Delta}_k(\widetilde{x}_k) \right| < \left| \Delta_k(x_k) \right| = \max_{x>0} \left| \Delta_k(x) \right|$$

with x_k and \tilde{x}_k given by (15) and (20), respectively. But

$$\left|\widetilde{\Delta}_k(x)\right| > \left|\Delta_k(x)\right| \quad \text{for } x > \widetilde{x}_k,$$

and

$$2x_k < \widetilde{x}_k < \min\left(1, \frac{1}{\sqrt{c_k^*(1 - (4c_k^*)^{-2})}}\right).$$

The approximation errors $\widetilde{\Delta}_k$ are depicted in Figure 3. They look similar to the errors Δ_k in Section 4. For a direct comparison, some error functions Δ_k and $\widetilde{\Delta}_k$ are displayed simultaneously in Figure 4. One sees clearly that $|\Delta_k| \geq |\widetilde{\Delta}_k|$ on $[0, \widetilde{x}_k]$, while $|\Delta_k| < |\widetilde{\Delta}_k|$ on $(\widetilde{x}_k, \infty)$.

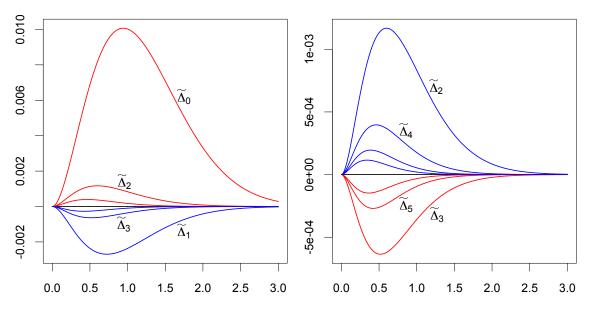


Figure 3: Approximation errors $\widetilde{\Delta}_k$ for k = 0, 1, ..., 5 (left) and k = 2, 3, ..., 9 (right).

Proof of Theorem 2. Our previous considerations show already that $\widetilde{\Delta}_k > 0$ for even k and $\widetilde{\Delta}_k < 0$ for odd k on $(0, \infty)$. To verify that $\widetilde{\Delta}_k > \widetilde{\Delta}_{k+2}$ for even k and $\widetilde{\Delta}_k < \widetilde{\Delta}_{k+2}$ for odd k, we have show that for any integer $k \geq 0$ and k > 0,

(21)
$$\sqrt{c_k^*} + (c_k - k)x < x + \frac{k+1}{x + \frac{k+2}{\sqrt{c_{k+2}^*} + (c_{k+2}^* - k - 2)x}}.$$

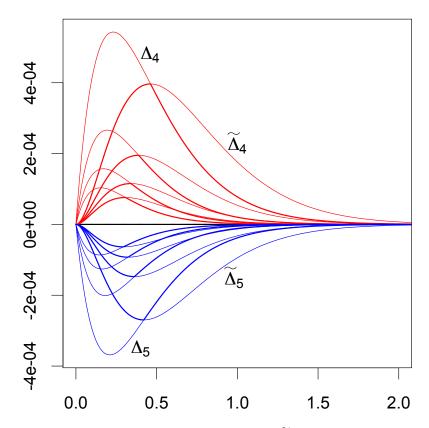


Figure 4: Approximation errors Δ_k and $\widetilde{\Delta}_k$ for $k = 4, 5, \dots, 11$.

But this is equivalent to

$$0 < \frac{k+1-c_k^*}{\sqrt{c_k^*}}x + \frac{k+1}{\sqrt{c_k^*}x + \frac{(k+2)\sqrt{c_k^*}}{\sqrt{c_{k+2}^*} + (c_{k+2}^* - k - 2)x}} - 1$$

$$= \frac{k+1-c_k^*}{\sqrt{c_k^*}}x + \frac{1}{\frac{\sqrt{c_k^*}}{k+1}x + \frac{\sqrt{c_{k+2}^*}}{\sqrt{c_{k+2}^*} + (c_{k+2}^* - k - 2)x}} - 1$$

according to (12). With

$$\alpha_k := \frac{k+1-c_k^*}{\sqrt{c_k^*}}, \quad \beta_k := \frac{\sqrt{c_k^*}}{k+1} \quad \text{and} \quad \gamma_k := \frac{c_{k+2}^*-k-2}{\sqrt{c_{k+2}^*}},$$

we may rewrite (22) as

$$\alpha_{k} x + \frac{1}{\beta_{k} x + \frac{1}{\gamma_{k} x + 1}} - 1 = \alpha_{k} x + \frac{\gamma_{k} x + 1}{\beta_{k} \gamma_{k} x^{2} + \beta_{k} x + 1} - 1$$

$$= \frac{\alpha_{k} \beta_{k} \gamma_{k} x^{3} + (\alpha_{k} - \gamma_{k}) \beta_{k} x^{2} + (\alpha_{k} + \gamma_{k} - \beta_{k}) x}{\beta_{k} \gamma_{k} x^{2} + \beta_{k} x + 1}.$$

But it follows from $k + 1/2 < c_k^* < k + 1$ and $c_{k+2}^* > k + 5/2$ that $\alpha_k, \beta_k, \gamma_k > 0$, and

$$\alpha_k - \gamma_k = \frac{k+1-c_k^*}{\sqrt{c_k^*}} - \frac{(k+2)^2(k+1)^{-2}c_k^* - k - 2}{(k+2)(k+1)^{-1}\sqrt{c_k^*}}$$

$$\sim k+1-c_k^* - (k+2)(k+1)^{-1}c_k^* + k + 1$$

$$= 2k+2 - (2k+3)(k+1)^{-1}c_k^*$$

$$\sim \frac{(k+1)^2}{k+3/2} - c_k^*$$

$$= k+1/2 + \frac{1}{4k+6} - c_k^*.$$

For $k \ge 1$, 4k + 6 < 8k + 4 = 8(k + 1/2), so $\alpha_k - \gamma_k > 0$ by Lemma 3, while $\alpha_0 - \gamma_0 \sim 2/3 - 2/\pi > 0$. Moreover,

$$\alpha_k + \gamma_k - \beta_k = \frac{k+1-c_k^* + (k+2)(k+1)^{-1}c_k^* - (k+1)}{\sqrt{c_k^*}} - \beta_k$$
$$= \frac{\sqrt{c_k^*}}{k+1} - \beta_k = 0.$$

Thus we have verified (21).

Concerning the comparison of $\widetilde{\Delta}_k$ and Δ_k , note that

$$\sqrt{c_k^*} + (c_k - k)x \ge \sqrt{c_k^* + (x/2)^2} + x/2$$

if, and only if,

$$\sqrt{c_k^* + (c_k^* - k - 1/2)x} \ge \sqrt{c_k^* + x^2/4}$$

For $x \geq 0$, the latter inequality is equivalent to

$$x \leq \frac{2\sqrt{c_k^*}(c_k^* - k - 1/2)}{1/4 - (c_k^* - k - 1/2)^2} = \frac{2\sqrt{c_k^*}}{(c_k^* - k)(k + 1 - c_k^*)} = \widetilde{x}_k,$$

and we know already that \widetilde{x}_k is the unique maximizer of $|\widetilde{\Delta}_k|$. On the other hand, we also know that the unique maximizer of $|\Delta_k|$ is given by (15), and

$$\frac{x_k}{\widetilde{x}_k} = \sqrt{1/4 - (c_k^* - k - 1/2)^2} < 1/2.$$

This shows that

$$\max_{x>0} \left| \Delta_k(x) \right| \ = \ \left| \Delta_k(x_k) \right| \ > \ \left| \Delta_k(\widetilde{x}_k) \right| \ = \ \left| \widetilde{\Delta}_k(\widetilde{x}_k) \right| \ = \ \max_{x>0} \left| \widetilde{\Delta}_k(x) \right|.$$

It remains to show that \tilde{x}_k is smaller than one and smaller than the reciprocal of $\sqrt{c_k^*} (1 - (4c_k^*)^{-2})$. On the one hand, $\tilde{x}_0 = \sqrt{\pi/2}(4-\pi)/(\pi-2) < 1$. On the other hand, it follows from Lemma 3 that $c_k^* < k + 1/2 + (8c_k^*)^{-1}$, so

$$\widetilde{x}_k < \frac{2\sqrt{c_k^*(8c_k^*)^{-1}}}{1/4 - (8c_k^*)^{-2}} = \frac{1}{\sqrt{c_k^*(1 - (4c_k^*)^{-2})}}.$$

Note also that the latter bound is strictly decreasing in $c_k^* > 1/2$. Since $c_1^* > 3/2$, it is strictly smaller than $36/35\sqrt{2/3} < 0.82$ for all $k \ge 1$.

6 New Bounds Involving Exponentials

As a final type of approximation, consider h_k as in Lemma 1 with

$$g_k(x) := x + \sqrt{c_k^*} \exp(-\delta_k x)$$

for some $\delta_k > 0$ to be specified later. Here

$$g_{k}(x)^{2} - xg_{k}(x) - k - g'_{k}(x)$$

$$= \sqrt{c_{k}^{*}} \exp(-\delta_{k}x) \left(x + \sqrt{c_{k}^{*}} \exp(-\delta_{k}x)\right) - (k+1) + \delta_{k}\sqrt{c_{k}^{*}} \exp(-\delta_{k}x)$$

$$\sim \delta_{k} + x + \sqrt{c_{k}^{*}} \exp(-\delta_{k}x) - \frac{k+1}{\sqrt{c_{k}^{*}}} \exp(\delta_{k}x)$$

$$=: f_{k}(x).$$

Note that

$$f_{k}(0) = \delta_{k} - \frac{k+1-c_{k}^{*}}{\sqrt{c_{k}^{*}}},$$

$$f'_{k}(x) = 1 - \delta_{k} \Big(\sqrt{c_{k}^{*}} \exp(-\delta_{k}x) + \frac{k+1}{\sqrt{c_{k}^{*}}} \exp(\delta_{k}x) \Big),$$

$$f''_{k}(x) = \delta_{k}^{2} \Big(\sqrt{c_{k}^{*}} \exp(-\delta_{k}x) - \frac{k+1}{\sqrt{c_{k}^{*}}} \exp(\delta_{k}x) \Big)$$

$$\leq \frac{\delta_{k}^{2}}{\sqrt{c_{k}^{*}}} (c_{k}^{*} - k - 1) < 0.$$

Thus f_k is strictly concave on $[0,\infty)$ with $\lim_{x\to\infty} f_k(x) = -\infty$. Setting

(23)
$$\delta_k := \frac{k+1-c_k^*}{\sqrt{c_k^*}} = \sqrt{c_{k+1}^*} - \sqrt{c_k^*}$$

leads to $f_k(0) = 0$ and, by Lemma 3,

$$f'_k(0) = 1 - \frac{(k+1-c_k^*)(k+1+c_k^*)}{c_k^*}$$

$$= 1 + c_k^* - \frac{(k+1)^2}{c_k^*}$$

$$> k+3/2 + (8(k+1))^{-1} - \frac{(k+1)^2}{k+1/2 + (8(k+1))^{-1}}$$

$$= \frac{1}{64(k+1)^2(k+1/2) + 8(k+1)} > 0.$$

Hence, with this choice of δ_k , the function g_k satisfies the conditions of Lemma 2. Note also that

$$(x + \sqrt{c_k^*} \exp(-\delta_k x)) - (\sqrt{c_k^*} + (c_k^* - k)x) = \sqrt{c_k^*} (\delta_k x + \exp(-\delta_k x) - 1) > 0.$$

Hence the resulting bounds for $1 - \Phi$ are strictly better than the ones in Section 5.

Theorem 3. Let

$$\widehat{h}_0(x) := x + \sqrt{2/\pi} \exp(-\delta_0 x), \quad \widehat{h}_1(x) := x + \frac{1}{x + \sqrt{\pi/2} \exp(-\delta_1 x)}$$

and, for integers $k \geq 2$,

$$\widehat{h}_k(x) := x + \frac{1}{x + \frac{2}{x + \frac{k}{x + \sqrt{c_k^*} \exp(-\delta_k x)}}},$$

where $\delta_k := \sqrt{c_{k+1}^*} - \sqrt{c_k^*}$. Then the approximation errors $\widehat{\Delta}_k := \phi/\widehat{h}_k - (1 - \Phi)$ and $\widetilde{\Delta}_k$ (as in Theorem 2) satisfy the following inequalities on $(0, \infty)$:

$$\widehat{\Delta}_0 > \widehat{\Delta}_2 > \widehat{\Delta}_4 > \dots > 0$$
 and $\widehat{\Delta}_1 < \widehat{\Delta}_3 < \widehat{\Delta}_5 < \dots < 0$.

Moreover,

$$|\widehat{\Delta}_k| < |\widetilde{\Delta}_k|.$$

Figure 5 shows the approximation errors $\widehat{\Delta}_k$ for k = 0, 2, ..., 9. Table 1 contains some values of the maximum of $|\Delta_k|$ and $|\widehat{\Delta}_k|$, rounded up to four significant digits. Although the bounds ϕ/\widehat{h}_k are much better than ϕ/h_k or ϕ/\widetilde{h}_k in terms of maximal error, note that $|\Delta_k(x)| < |\widehat{\Delta}_k(x)|$ for sufficiently large x > 0. Precisely, $|\Delta_k(x)| < |\widehat{\Delta}_k(x)|$ if, and only if,

$$\exp(\delta_k x) > \frac{\sqrt{c_k^* + (x/2)^2} + x/2}{\sqrt{c_k^*}},$$

and numerical experiments show that this is true for $x \ge 3.2$ if k = 0 and $x \ge 3$ if $k \ge 1$.

Proof of Theorem 3. We only have to show that $\widehat{\Delta}_k > \widehat{\Delta}_{k+2}$ for even k and $\widehat{\Delta}_k < \widehat{\Delta}_{k+2}$ for odd k on $(0, \infty)$. This means that for any integer $k \geq 0$ and x > 0,

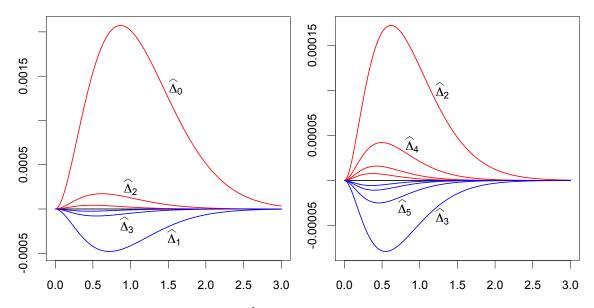


Figure 5: Approximation errors $\widehat{\Delta}_k$ for k = 0, 1, ..., 5 (left) and k = 2, 3, ..., 9 (right).

the difference

$$x + \frac{k+1}{x + \frac{k+2}{g_{k+2}(x)}} - g_k(x) = \frac{(k+1)g_{k+2}(x)}{xg_{k+2}(x) + k + 2} - (g_k(x) - x)$$

$$= \frac{(k+1)g_{k+2}(x)}{xg_{k+2}(x) + k + 2} - \sqrt{c_k^*} \exp(-\delta_k x)$$

$$\sim \sqrt{c_{k+1}^*} \exp(\delta_k x)g_{k+2}(x) - xg_{k+2}(x) - (k+2)$$

$$= \sqrt{c_{k+1}^*} \exp(\delta_k x)x - \sqrt{c_{k+2}^*} \exp(-\delta_{k+2}x)x - x^2$$

$$+ (k+2) \Big(\exp((\delta_k - \delta_{k+2})x) - 1 \Big)$$

is strictly positive. Note that we utilized (11) twice. Note also that

$$\delta_{k} - \delta_{k+2} = \sqrt{c_{k+1}^{*}} - \sqrt{c_{k}^{*}} - \sqrt{c_{k+3}^{*}} + \sqrt{c_{k+2}^{*}}$$

$$= \sqrt{c_{k+1}^{*}} - \frac{k+1}{k+2} \sqrt{c_{k+2}^{*}} - \frac{k+3}{k+2} \sqrt{c_{k+1}^{*}} + \sqrt{c_{k+2}^{*}}$$

$$= \frac{\sqrt{c_{k+2}^{*}} - \sqrt{c_{k+1}^{*}}}{k+2} = \frac{\delta_{k+1}}{k+2}$$

k	$\left \max_{x>0} \left \widehat{\Delta}_k(x) \right \right $	$\left \max_{x>0} \left \Delta_k(x) \right \right $	$\max_{x \ge 1} \left \Delta_k(x) \right $	$\max_{x \ge 2} \left \Delta_k(x) \right $	$\left \max_{x \ge 3} \left \Delta_k(x) \right \right $
0	$2.074 \cdot 10^{-3}$	$1.571 \cdot 10^{-2}$	$9.194 \cdot 10^{-3}$	$9.374 \cdot 10^{-4}$	$3.550 \cdot 10^{-5}$
1	$4.796 \cdot 10^{-4}$	$3.820 \cdot 10^{-3}$	$1.606 \cdot 10^{-3}$	$1.041 \cdot 10^{-4}$	$2.612 \cdot 10^{-6}$
2	$1.723 \cdot 10^{-4}$	$1.622 \cdot 10^{-3}$	$4.687 \cdot 10^{-4}$	$1.896 \cdot 10^{-5}$	$3.175 \cdot 10^{-7}$
3	$7.888 \cdot 10^{-5}$	$8.735 \cdot 10^{-4}$	$1.764 \cdot 10^{-4}$	$4.591 \cdot 10^{-6}$	$5.226 \cdot 10^{-8}$
4	$4.214 \cdot 10^{-5}$	$5.433 \cdot 10^{-4}$	$7.775 \cdot 10^{-5}$	$1.342 \cdot 10^{-6}$	$1.059 \cdot 10^{-8}$
5	$2.499 \cdot 10^{-5}$	$3.685 \cdot 10^{-4}$	$3.814 \cdot 10^{-5}$	$4.480 \cdot 10^{-7}$	$2.497 \cdot 10^{-9}$
6	$1.599 \cdot 10^{-5}$	$2.663 \cdot 10^{-4}$	$2.023 \cdot 10^{-5}$	$1.655 \cdot 10^{-7}$	$6.625 \cdot 10^{-10}$
7	$1.082 \cdot 10^{-5}$	$2.010 \cdot 10^{-4}$	$1.138 \cdot 10^{-5}$	$6.616 \cdot 10^{-8}$	$1.932 \cdot 10^{-10}$

Table 1: Maximal approximation errors.

by (12). Hence dividing (24) by x yields

$$\sqrt{c_{k+1}^*} \exp(\delta_k x) - \sqrt{c_{k+2}^*} \exp(-\delta_{k+2} x) - x
+ (k+2) \left(\exp\left(\frac{\delta_{k+1} x}{k+2}\right) - 1 \right) / x
= \sqrt{c_{k+1}^*} \left(\exp(\delta_k x) - 1 \right) - \sqrt{c_{k+2}^*} \left(\exp(-\delta_{k+2} x) - 1 \right) - x
+ (k+2) \left(\exp\left(\frac{\delta_{k+1} x}{k+2}\right) - 1 - \frac{\delta_{k+1} x}{k+2} \right) / x
> \sqrt{c_{k+1}^*} \left(\exp(\delta_k x) - 1 \right) - \sqrt{c_{k+2}^*} \left(\exp(-\delta_{k+2} x) - 1 \right) - x =: J_k(x).$$

To verify that $J_k(x) > 0$ for all x > 0, note that $J_k(0) = 0$ and

$$J'_{k}(0) = \sqrt{c_{k+1}^{*}} \, \delta_{k} + \sqrt{c_{k+2}^{*}} \, \delta_{k+2} - 1$$

$$= (c_{k+1}^{*} - k - 1) + (k + 3 - c_{k+2}^{*}) - 1$$

$$= c_{k+1}^{*} - c_{k+2}^{*} + 1$$

$$> \frac{1}{8(k+2)} - \frac{1}{8(k+5/2)}$$

$$= \frac{1}{16(k+2)(k+5/2)} > 0$$

by Lemma 3. Finally,

$$J_k''(x) = \sqrt{c_{k+1}^*} \, \delta_k^2 \exp(\delta_k x) - \sqrt{c_{k+2}^*} \, \delta_{k+2}^2 \exp(-\delta_{k+2} x)$$

$$> \sqrt{c_{k+1}^*} \, \delta_k^2 - \sqrt{c_{k+2}^*} \, \delta_{k+2}^2$$

$$= (c_{k+1}^* - k - 1) \delta_k - (k + 3 - c_{k+2}^*) \delta_{k+2}$$

$$> \delta_k / 2 - \delta_{k+2} / 2 > 0,$$

7 Alternative Representations

In this section we describe briefly representations of our approximations in terms of simple fractions rather than continued fractions. This material is rather standard, and we refer to Kouba (2006) for deeper connections with Hermite polynomials.

Lemma 4. Let $h_0, h_1, h_2, ...$ be constructed as in Lemma 1. Define polynomials via $P_0(x) := 1$, $P_1(x) := x$, $Q_0(x) := 0$, $Q_1(x) := 1$ and inductively, for k = 2, 3, 4, ...,

$$P_k(x) := (k-1)P_{k-2}(x) + xP_{k-1}(x),$$

$$Q_k(x) := (k-1)Q_{k-2}(x) + xQ_{k-1}(x).$$

Then for arbitrary $k \ge 1$ and x > 0,

$$h_k(x) = \frac{kP_{k-1}(x) + P_k(x)g_k(x)}{kQ_{k-1}(x) + Q_k(x)g_k(x)}.$$

In particular, if $g_k(x) = x$, then $h_k(x) = P_{k+1}(x)/Q_{k+1}(x)$.

Table 2 contains a list of the polynomials P_k, Q_k for $0 \le k \le 8$. Suppose that $g_k(x) = x + G_k(x)$ for some $G_k : [0, \infty) \to (0, \infty)$, for instance,

$$G_k(x) := \sqrt{c_k^* + (x/2)^2} - x/2 = \frac{c_k^*}{\sqrt{c_k^* + (x/2)^2} + x/2}$$
 in Section 4,

$$G_k(x) := \sqrt{c_k^*} \exp\left(-\left(\sqrt{c_{k+1}^*} - \sqrt{c_k^*}\right)x\right)$$
 in Section 6.

Then

$$h_k = \frac{P_{k+1} + P_k G_k}{Q_{k+1} + Q_k G_k}$$
 on $[0, \infty)$.

For instance,

$$h_2(x) = \frac{x^3 + 3x + (x^2 + 1)G_2(x)}{x^2 + 2 + xG_2(x)},$$

$$h_3(x) = \frac{x^4 + 6x^2 + 3 + (x^3 + 3x)G_3(x)}{x^3 + 5x + (x^2 + 2)G_3(x)},$$

$$h_4(x) = \frac{x^5 + 10x^3 + 15x + (x^4 + 6x^2 + 3)G_4(x)}{x^4 + 9x^2 + 8 + (x^3 + 5x)G_4(x)},$$

$$h_5(x) = \frac{x^6 + 15x^4 + 45x^2 + 15 + (x^5 + 10x^3 + 15x)G_5(x)}{x^5 + 14x^3 + 33x + (x^4 + 9x^2 + 8)G_5(x)}.$$

$\lceil k \rceil$		$P_k(x) = \sum_j a_j x^j$							$Q_k(x) = \sum_j b_j x^j$								
	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	b_0	b_1	b_2	b_3	b_4	b_5	b_6	b_7
0	1									0							
1	0	1								1							
2	1	0	1							0	1						
3	0	3	0	1						2	0	1					
4	3	0	6	0	1					0	5	0	1				
5	0	15	0	10	0	1				8	0	9	0	1			
6	15	0	45	0	15	0	1			0	33	0	14	0	1		
7	0	105	0	105	0	21	0	1		48	0	87	0	20	0	1	
8	105	0	420	0	210	0	28	0	1	0	279	0	185	0	27	0	1

Table 2: Auxiliary polynomials P_k, Q_k for $0 \le k \le 8$.

Proof of Lemma 4. Note first that $h_k(x)$ may be written as

$$h_k(x) = \frac{A_k(x) + P_k(x)g_k(x)}{B_k(x) + Q_k(x)g_k(x)}$$

with certain polynomials A_k, P_k, B_k, Q_k . Indeed,

$$h_0(x) = \frac{0+1 \cdot g_0(x)}{1+0 \cdot g_0(x)}, \quad \text{so } [A_0(x), P_0(x), B_0(x), Q_0(x)] = [0, 1, 1, 0],$$

$$h_1(x) = \frac{1+xg_1(x)}{0+1 \cdot g_1(x)}, \quad \text{so } [A_1(x), P_1(x), B_1(x), Q_1(x)] = [1, x, 0, 1].$$

For $k \ge 2$, let $g_{k-1}(x) := x + k/g_k(x) = (k + xg_k(x))/g_k(x)$. Then

$$h_k(x) = h_{k-1}(x) = \frac{A_{k-1}(x)g_k(x) + P_{k-1}(x)(k + xg_k(x))}{B_{k-1}(x)g_k(x) + Q_{k-1}(x)(k + xg_k(x))}$$
$$= \frac{kP_{k-1}(x) + (A_{k-1}(x) + xP_{k-1}(x))g_k(x)}{kQ_{k-1}(x) + (B_{k-1}(x) + xQ_{k-1}(x))g_k(x)},$$

i.e.

$$A_k(x) = kP_{k-1}(x)$$
 and $P_k(x) = A_{k-1}(x) + xP_{k-1}(x)$, $B_k(x) = kQ_{k-1}(x)$ and $Q_k(x) = B_{k-1}(x) + xQ_{k-1}(x)$.

Since $A_1(x) = 1 \cdot P_0(x)$ and $B_1(x) = 1 \cdot Q_0(x)$, we may write

$$h_k(x) = \frac{kP_{k-1}(x) + P_k(x)g_k(x)}{kQ_{k-1}(x) + Q_k(x)g_k(x)}$$
 for $k \ge 1$,

where

$$P_k(x) = (k-1)P_{k-2}(x) + xP_{k-1}(x)$$
 and
$$Q_k(x) = (k-1)Q_{k-2}(x) + xQ_{k-1}(x) \text{ for } k = 2, 3, 4, \dots$$

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