

## Multiple precision evaluation of the Airy Ai function with reduced cancellation

Sylvain Chevillard, Marc Mezzarobba

### ▶ To cite this version:

Sylvain Chevillard, Marc Mezzarobba. Multiple precision evaluation of the Airy Ai function with reduced cancellation. 21st IEEE Symposium on Computer Arithmetic, 2013, Austin, TX, United States. hal-00767085v1

## HAL Id: hal-00767085 https://inria.hal.science/hal-00767085v1

Submitted on 19 Dec 2012 (v1), last revised 28 Apr 2013 (v2)

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Multiple precision evaluation of the Airy Ai function with reduced cancellation

Sylvain Chevillard Inria, Apics Project-Team, Sophia Antipolis, France sylvain.chevillard@inria.fr

Abstract—The series expansion at the origin of the Airy function Ai(x) is alternating and hence problematic to evaluate for x > 0 due to cancellation. Based on a method recently proposed by Gawronski, Müller, and Reinhard, we exhibit two functions F and G, both with nonnegative Taylor expansions at the origin, such that Ai(x) = G(x)/F(x). The sums are now well-conditioned, but the Taylor coefficients of G turn out to obey an ill-conditioned three-term recurrence. We use the classical Miller algorithm to overcome this issue. We bound all errors and our implementation allows an arbitrary and certified accuracy, that can be used, e.g., for providing correct rounding in arbitrary precision.

*Index Terms*—Special functions; algorithm; numerical evaluation; arbitrary precision; Miller method; asymptotics; correct rounding; error bounds.

Many mathematical functions (e.g., trigonometric functions, erf, Bessel functions) have a Taylor series of the form

$$y(x) = \sum_{n=0}^{\infty} y_n x^n, \quad y_n \approx (-1)^n \frac{\alpha^n}{n!^{\kappa}}, \quad \alpha, \kappa > 0.$$
(1)

For large x > 0, the computation in finite precision arithmetic of such a sum is notoriously prone to *catastrophic cancellation*. Indeed, the terms  $|y_n x^n|$  are first growing before the series "starts to converge" when  $n^{\kappa} \ge \alpha x$ . In particular, when  $n^{\kappa} \approx \alpha x$ , the terms  $y_n x^n$  usually get much larger than y(x). Eventually, their leading bits cancel out while lower-order bits that actually contribute to the first significant digits of the result get lost in roundoff errors.

This cancellation phenomenon makes the direct computation by Taylor series impractical for large values of x. Often, the function y(x) admits an asymptotic expansion as  $x \to +\infty$  that can be used very effectively to obtain numerical approximations when x is large, but might not provide enough accuracy (at least without resorting to sophisticated resummation methods) for intermediate values of x.

In the case of the error function erf(x), a classical trick going back at least to Stegun and Zucker [17] is to compute erf(x) as G(x)/F(x) where  $F(x) = e^{x^2}$  and [1, Eq. 7.6.2]

$$G(x) = e^{x^2} \operatorname{erf}(x) = \frac{2x}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{2^n}{1 \cdot 3 \cdots (2n+1)} x^{2n}.$$
 (2)

The benefit of this transformation is that *F* and *G* are power series with nonnegative coefficients, and can thus be computed without cancellation. Algorithms based on (2) tend to be competitive in some range a < x < b where *x* is large enough for cancellation to be problematic but small enough to make the use of asymptotic expansions at infinity inconvenient. Note

Marc Mezzarobba

Inria, LIP (CNRS-ENS-Inria-UCBL), ENS de Lyon, France marc@mezzarobba.net

that the obvious way to compute  $y(x) = e^{-x}$  for x > 0 fits into the same frame, now with G(x) = 1 and  $F(x) = e^x$ .

Gawronski, Müller and Reinhard [8], [14] provide elements to understand where these rewritings "come from". They relate the amount of cancellation in the summation of a series (1) to the shape of the Phragmén-Lindelöf indicator of y, a classical tool from the theory of entire functions [10]. This description allows them to state criteria for choosing auxiliary series suitable for the evaluation of a given entire function in a given sector of the complex plane. They apply their method (called the "GMR method" in what follows) to obtain "reduced cancellation" evaluation algorithms for the error function and other related functions in various sectors.

In this article, we are interested in the evaluation for positive x of the Airy function Ai [1, Chap. 9]. The function Ai(x) satisfies the linear ordinary differential equation (LODE)

$$\operatorname{Ai}''(x) - x\operatorname{Ai}(x) = 0 \tag{3}$$

with initial values

Ai(0) = 
$$A := 3^{-2/3} \Gamma(\frac{2}{3})^{-1}$$
, Ai'(0) =  $-B := -3^{-1/3} \Gamma(\frac{1}{3})^{-1}$ .

The classical existence theorem for LODE with complex analytic coefficients implies that Ai(x) is an entire function; and solving (3) by the method of power series yields the Taylor expansion  $Ai(x) = Af(x^3) - Bxg(x^3)$ , where

$$f(x) = \sum_{n=0}^{\infty} \frac{1 \cdot 4 \cdots (3n-2)}{(3n)!} x^n, \quad g(x) = \sum_{n=0}^{\infty} \frac{2 \cdot 5 \cdots (3n-1)}{(3n)!} x^n.$$

Observe that while f and g are easy enough to evaluate individually, the difference  $Af(x^3)-Bxg(x^3)$  causes catastrophic cancellation when computed in approximate arithmetic.

Using the GMR method, we derive a reduced cancellation algorithm for computing Ai(x). To our best knowledge, our algorithm for evaluating Ai(x) is new, and is the most efficient multiple-precision evaluation of Ai(x) when x is neither too small nor too large, while the precision is not large enough to make methods based on binary splitting [4] competitive.

Besides the new application, the main difference between the present article and the work of Gawronski *et al.* is our setting of multiple precision arithmetic "à la MPFR [7]". Specifically, on the one hand, we are interested in *arbitrary precision* arithmetic rather than machine precision only. This makes it impossible, for instance, to tabulate the coefficients of auxiliary functions when these turn out to be hard to compute. Also, we are looking for *rigorous error bounds* instead of experimental

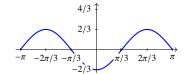


Figure 1. The indicator function h of Ai.

error estimates. On the other hand, we restrict ourselves to numerical evaluation on a half line instead of a complex sector.

This article focuses on providing a complete algorithm in the specific case of Ai(x), x > 0. Yet, it should also be seen a *case study*, part of an effort to understand what the GMR method can bring in the context of multiple precision computation, and, perhaps more importantly, how general and systematic it can be made. We discuss this last point further in Sec. VIII.

The rest of the text is organized as follows. In Sec. I, we use the GMR method to choose the auxiliary functions F and G. Then, in Sec. II and III, we derive a few mathematical properties of these functions, including recurrences for their series expansions and various bounds. Sections IV to VI contain the details of our algorithm and its error analysis. Finally, in Sec. VII, we briefly describe our implementation of the algorithm and present preliminary experimental results.

#### I. The GMR method

We now review the GMR method and apply it to obtain candidate auxiliary series for the evaluation of the Ai function. Since the method itself is not crucial for our results, we summarize it in intuitive terms and refer the reader to the original works [8], [14] for more careful statements.

The starting point of the GMR method is the following observation. Let  $y(z) = \sum_{n\geq 0} y_n z^n$  be an entire function. Assume that we have, in some intentionally vague sense,

$$y(re^{i\theta}) \approx \exp(h(\theta)r^{\rho})$$
 (4)

for large r. (To make things precise, we would assume that y has finite order  $\rho$ , and that h is its *indicator function* with respect to  $\rho$  [10].)

We consider the computation of y(z) in floating-point arithmetic using its series expansion. It is well-known [5] that, if the sum is performed in floating-point arithmetic of precision *t*, the relative error between y(z) and the computed sum is roughly given by  $(\sum_{n\geq 0} |y_n z^n|)/|y(z)|$ . The sum  $\sum_{n\geq 0} |y_n z^n|$ is larger than  $\max_{n\geq 0} |y_n z^n|$ , and usually of the same order of magnitude. Therefore, the number of significant digits "lost by cancellation" is roughly

$$\lg(\max|y_n z^n|) - \lg|y(z)|.$$

Denote  $M(r) = \sup_{|z|=r} |y(z)|$  for all r > 0. Cauchy's formula implies  $\max_n(|y_n|r^n) \le M(r)$ , and under a suitable version of hypothesis (4), one can actually show that  $\max_n(|y_n|r^n) \approx M(r)$ . Hence, the loss of precision by cancellation in the evaluation of  $y(re^{i\theta})$  is about

$$\lg \frac{M(r)}{|y(re^{i\theta})|} \approx [(\max h) - h(\theta)] r^{\rho}.$$

For instance, when the  $y_n$  all have the same complex argument, the maximum of *h* is reached for  $\theta = 0$ , in accordance with the fact that the sum is optimally conditioned.

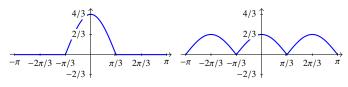


Figure 2. Indicator functions for F (left) and G (right).

In the case of the Airy Ai function, the following asymptotic equivalent holds as z tends to complex infinity in any open sector that avoids the negative real axis [1, Eq. 9.7.5]:

$$\operatorname{Ai}(z) \sim \widetilde{\operatorname{Ai}}(z) := \frac{\exp(-\frac{2}{3}z^{3/2})}{2\sqrt{\pi}z^{1/4}}.$$
 (5)

Additionally, Ai(x) is bounded for x < 0. Hence, we may take  $\rho = 3/2$  and

$$h(\theta) = -\frac{2}{3}\cos(\frac{3}{2}\theta), \qquad -\pi < \theta \le \pi \tag{6}$$

(see Figure 1). The loss of precision is roughly proportional to  $1 + \cos(\frac{3}{2}\theta)$ . It is minimal in the directions of fastest growth  $\theta = \pm \frac{2}{3}\pi$ , and maximal for  $\theta = 0$ .

If now two entire functions y and F both satisfy conditions of the form (4) with the same  $\rho$  but different h (say  $h_y$  and  $h_F$ , respectively), we may expect that

$$G(z) = F(z)y(z) \approx \exp([h_y(\theta) + h_F(\theta)]z^{\rho}).$$
(7)

The GMR method consists in reducing the summation of the series *y* for *z* in some given sector to that of an *auxiliary series* F(z) and a *modified series* G(z) related by (7). The value of y(z) is then recovered as G(z)/F(z). The auxiliary series is chosen, based on the shape of  $h_y$ , so that both  $h_F$  and  $h_G = h_y + h_F$  take values close to their maximum in the sector of interest.

Gawronski *et al.* usually take  $F(z) = \exp(az^{\rho})$  and search for a value of *a* that makes  $(\max h_G) - h_G$  as small as possible on a whole complex sector. The choice of exponentials as auxiliary series is not appropriate in the case of Ai, since  $\exp(z^{\rho})$  is an entire function of *z* only for integer  $\rho$ .

However, as we are interested in one direction only, we can easily build a suitable auxiliary series from Ai itself. Indeed, we may "shift" the indicator function of Ai by  $2\pi/3$  to the left or to the right by changing z to  $j^{\pm 1}z$ , where  $j = e^{2\pi i/3}$ . (Note that this is *not* the same as changing  $\theta$  to  $\theta \pm \frac{2}{3}\pi$  in (6).) When we add such a shifted indicator to the original  $h_{Ai}$ , one of the humps of the curve cancels out with the valley in the middle.

Using this idea, we set

$$F(x) = \operatorname{Ai}(jx)\operatorname{Ai}(j^{-1}x), \quad G(x) = F(x)\operatorname{Ai}(x).$$
 (8)

The indicator functions of F and G are pictured on Figure 2. Based on their shapes, we expect that both series are optimally conditioned on the positive real axis. We shall prove that this is indeed the case in the next two sections.

This second method of constructing auxiliary series seems to be new, and applies to many cases. For instance, applying it to the error function leads to

$$F(x) = -i \operatorname{erf} ix = \frac{2x}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{1 \cdot 3 \cdots (2n-1)}{(2n+1)!} 2^n x^{2n},$$
$$G(x) = F(x) \operatorname{erf} x = \frac{8x^2}{\pi} \sum_{n=0}^{\infty} \frac{2 \cdot 4 \cdots (4n)}{(4n+2)!} 4^n x^{4n},$$

a slightly worse alternative to (2). The advantage of (2) comes from the fact that  $e^{x^2}$  is faster to evaluate than F(x).

#### II. The auxiliary series F

The functions F and G being chosen, we need to establish appropriate formulas to evaluate them, along with error bounds. Much of our analysis will be based on the following simple estimate [13, Chap. 4, §4.1], where  $\widetilde{Ai}$  is the leading term of the asymptotic expansion of Ai(z) at infinity from Eq. (5).

Lemma 1: The Airy function Ai satisfies

$$|\operatorname{Ai}(re^{i\theta})/\operatorname{Ai}(re^{i\theta}) - 1| \le \eta_1(\theta)r^{-3/2}, \qquad |\theta| < \pi,$$

where  $\eta_1(\theta) = \frac{5}{48} (\cos \frac{\theta}{2})^{-1/2}$ .

Now consider the power series expansion of F at the origin:

$$F(x) = \operatorname{Ai}(jx)\operatorname{Ai}(j^{-1}x) = \sum_{n=0}^{\infty} F_n x^n.$$
 (9)

*Proposition 1:* The coefficients  $F_n$  are positive and satisfy the two-term recurrence relation

$$(n+1)(n+2)(n+3)F_{n+3} - 2(2n+1)F_n = 0$$
(10)

with initial values

$$F_0 = 3^{-4/3} \Gamma(\frac{2}{3})^{-2}, \qquad F_1 = (2\sqrt{3}\pi)^{-1}, \qquad F_2 = 3^{-2/3} \Gamma(\frac{1}{3})^{-2}.$$

*Proof:* As a general fact, if two functions w and y each satisfy a linear homogeneous ODE with coefficients in  $\mathbb{Q}(x)$ , then their product wy satisfies an equation of the same class that can be explicitly computed [16, Sec. 6.4]. The functions Ai $(j^{\pm 1}x)$  satisfy the same differential equation (3) as Ai(x) itself. (In other words, the substitution  $x \mapsto j^{\pm 1}x$  leaves (3) unchanged.) Applying the procedure mentioned above to two copies of that equation yields  $F^{(3)}(x) - 4xF'(x) - 2F(x) = 0$ .

Similarly, when an analytic function *y* satisfies a homogeneous LODE over  $\mathbb{Q}(x)$ , we can compute a recurrence relation with coefficients in  $\mathbb{Q}(n)$  on the coefficients  $y_n$  of its power series expansion. In the case of *F*, we get (10). Finally, we compute the initial values  $F_1, F_2, F_3$  from the first few terms of the Taylor expansion of Ai(*x*):

$$F(x) = (A - Bjx + O(x^3))(A - Bj^{-1}x + O(x^3))$$
  
=  $A^2 - \frac{1}{2}ABx + B^2x^2 + O(x^3).$ 

It is then apparent from (10) that  $F_n > 0$  for all  $n \in \mathbb{N}$ .

Thus, the coefficients of F(x) obey a two-term recurrence whose coefficients do not vanish for  $n \ge 0$ . This allows one to compute them in a numerically stable way (see Sec. VI).

#### III. The modified series G

Recall that 
$$G(x) = \operatorname{Ai}(x) \operatorname{Ai}(jx) \operatorname{Ai}(j^{-1}x)$$
, and set

$$\widetilde{G}(x) = \widetilde{\operatorname{Ai}}(x)\widetilde{\operatorname{Ai}}(jx)\widetilde{\operatorname{Ai}}(j^{-1}x) = \frac{\exp(\frac{2}{3}x^{3/2})}{8\pi^{3/2}x^{3/4}}.$$
 (11)

*Proposition 2:* The function *G* is an entire function with power series expansion of the form  $G(z) = \sum_{n=0}^{\infty} G_n z^{3n}$ . The coefficient sequence  $(G_n)_{n \in \mathbb{N}}$  is determined from its first terms

$$G_0 = A^3 = \frac{1}{9\Gamma(2/3)^3}, \quad G_1 = \frac{A^3}{2} - B^3 = \frac{1}{18\Gamma(2/3)^3} - \frac{1}{3\Gamma(1/3)^3}$$
  
by the recurrence relation

$$(n+1)(3n+4)(3n+5)(n+2)G_{n+2}-10(n+1)^2G_{n+1}+G_n=0.$$
 (12)

*Proof:* First, observe that G(jz) = G(z) and  $G(\overline{z}) = \overline{G(z)}$ , so that the Taylor expansion of G at the origin is a power series in  $z^3$  with real coefficients. The same routine reasoning as in the proof of Prop. 1 yields the LODE

$$G^{(4)}(x) - 10xG''(x) - 10G'(x) + 9x^2G(x) = 0,$$

and from there the recurrence (12). The coefficients of (12) do not vanish for  $n \ge 0$ , so that the sequence  $G_n$  is indeed determined by  $G_0, G_1$ , and (12).

Nonzero solutions of (12) decrease roughly as  $n!^{-2}$  for large *n*. Setting  $c_n = n!^2 G_n$  yields the "normalized" recurrence (3n + 4)(3n + 5)

$$\frac{c_{n+1}(c_{n+1})(c_{n+2})}{(n+1)(n+2)}c_{n+2} - 10c_{n+1} + c_n = 0.$$
 (13)

Letting *n* go to infinity in the coefficients of (13), we get a limit recurrence with constant coefficients whose characteristic polynomial  $9\alpha^2 - 10\alpha + 1$  has two roots of distinct absolute value, namely  $\frac{1}{9}$  and 1. By the Perron-Kreuser theorem [20, Theorem B.10], it follows that any solution  $(v_n)_{n \in \mathbb{N}}$  of (12) satisfies  $v_{n+1}/v_n \sim \alpha n^{-2}$  with either  $\alpha = 1$  or  $\alpha = \frac{1}{9}$ . Solutions  $(v_n)$  such that  $v_{n+1}/v_n \sim \frac{1}{9n^2}$  are called *minimal* and form a subvector space of dimension 1 of the solutions of (12).

It turns out that  $(G_n)$  is a minimal solution of (12). But our analysis uses a bit more than the rough estimate  $G_n \approx n!^{-2}9^{-n}$ . Prop. 3 below provides a more precise estimate which implies the minimality. Before turning to it, we recall a standard bound on the tails of incomplete Gaussian integrals [1, Eq. 7.12.1] and state a second technical lemma.

*Lemma 2:* The complementary error function  $\operatorname{erfc} x = 1 - \operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt$  satisfies  $0 \le \operatorname{erfc} x \le \frac{1}{\sqrt{\pi}x} e^{-x^2}$  for x > 0. *Lemma 3:* The expression

$$I(r) = r^{9/8} \int_{r^{-5/8}}^{\pi/3} e^{\frac{2}{3}r^{3/2}(-1+\cos\frac{3\theta}{2})} \mathrm{d}\theta$$

satisfies  $0 \le I(r) \le 0.51$  for all  $r \ge 10$ .

*Proof:* We first use the inequality  $\cos(\frac{3}{2}\theta) \le 1 - \frac{9}{10}\theta^2$ (valid for  $0 \le \theta \le \pi/3$ ) followed by the change of variable  $\varphi = \sqrt{3/5} r^{3/4} \theta$  to get

$$I(r) \leq r^{9/8} \int_{r^{-5/8}}^{\pi/3} e^{-\frac{3}{3}r^{3/2}\theta^2} \mathrm{d}\theta = \frac{\sqrt{5}}{\sqrt{3}} r^{3/8} \int_{a(r)}^{b(r)} e^{-\varphi^2} \mathrm{d}\varphi,$$

where  $a(r) = \sqrt{3/5} r^{1/8}$  and  $b(r) = \frac{\pi}{\sqrt{15}} r^{3/4}$ . Now we have

$$\int_{a(r)}^{b(r)} e^{-\varphi^2} \mathrm{d}\varphi \le \int_{a(r)}^{\infty} e^{-\varphi^2} \mathrm{d}\varphi = \frac{\sqrt{\pi}}{2} \operatorname{erfc}\left(\frac{\sqrt{3}r^{1/8}}{\sqrt{5}}\right),$$

and, by Lemma 2,  $I(r) \leq \frac{5}{6}r^{1/4}e^{-\frac{2}{3}r^{1/4}}$ . This last bound is decreasing and less than 0.51 when r = 10.

The following proposition is the main result of this section and the starting point of much of the error analysis that follows. Though somewhat technical, the proof is mostly routine.

Proposition 3: The sequence  $(G_n)$  satisfies

$$G_n \sim \gamma_n = \frac{1}{4\sqrt{3}\pi 9^n n!^2}, \quad n \to \infty,$$

with relative approximation error  $|G_n/\gamma_n - 1| \le 2.4n^{-1/4}$ .

Notation 1: We write  $E(\varepsilon_1, \ldots, \varepsilon_n) = \sum_{\emptyset \neq I \subset [\![1,n]\!]} \prod_{i \in I} \varepsilon_i$ , so that, if  $|\theta_i| \leq \varepsilon_i$  for all *i*, then  $\prod_{i=1}^n (1 + \theta_i) = 1 + \theta$  with  $|\theta| \leq E(\varepsilon_1, \ldots, \varepsilon_n)$ . Note that we also have  $E(\alpha \varepsilon_1, \ldots, \alpha \varepsilon_n) \leq \alpha E(\varepsilon_1, \ldots, \varepsilon_n)$  for  $0 \leq \alpha \leq 1$ .

*Proof:* The proof is a standard application of the *saddle point method* [6, §VIII.3], which we work out in some detail in order to get an explicit error bound.

Start with the estimate from Lemma 1. Writing  $z = re^{i\theta}$  with  $r \ge 1$  and  $|\theta| < \pi/3$ , it follows that

$$|G(z)/\tilde{G}(z) - 1| \le \eta_2(\theta) r^{-3/2}$$
(14)

where  $\eta_2(\theta) = E(\eta_1(\theta), \eta_1(\theta + \frac{2\pi}{3}), \eta_1(\theta - \frac{2\pi}{3}))$ . Note that  $\eta_2(\theta)$  increases with  $|\theta|$ . Using the connection formula [1, Eq. 9.2.12]

$$\operatorname{Ai}(z) + j\operatorname{Ai}(jz) + j^{-1}\operatorname{Ai}(j^{-1}z) = 0,$$

and assuming now that  $0 \le \theta \le \pi/3$ , we see that  $|G(z)/\tilde{G}(z)|$  is bounded by

$$\begin{split} & \frac{\operatorname{Ai}(z)}{\widetilde{\operatorname{Ai}}(z)} \left| \left| \frac{\operatorname{Ai}(j^{-1}z)}{\widetilde{\operatorname{Ai}}(j^{-1}z)} \right| \left( \left| \frac{\widetilde{\operatorname{Ai}}(z)}{\widetilde{\operatorname{Ai}}(z)} \right| \left| \frac{\operatorname{Ai}(z)}{\widetilde{\operatorname{Ai}}(z)} \right| + \left| \frac{\widetilde{\operatorname{Ai}}(j^{-1}z)}{\widetilde{\operatorname{Ai}}(j^{-1}z)} \right| \right) \\ & \leq (1 + \eta_1(\theta)r^{-3/2})(1 + \eta_1(\theta - \frac{2\pi}{3})r^{-3/2}) \\ & \left( e^{-\frac{4}{3}\cos\frac{3\theta}{2}}(1 + \eta_1(\theta)r^{-\frac{3}{2}}) + 1 + \eta_1(\theta - \frac{2\pi}{3})r^{-\frac{3}{2}} \right). \end{split}$$

It follows that

 $|G(z)| \le 2.1 |\tilde{G}(z)|, \qquad |z| \ge 10.$  (15) By symmetry, these inequalities hold for  $-\pi/3 \le \theta \le 0$  too.

Now fix n > 10 and write

$$G_n = \frac{1}{2\pi i} \oint \frac{G(z)}{z^{3n+1}} dz = \frac{3}{2\pi} \frac{\tilde{G}(r)}{r^{3n}} I_1, \quad I_1 = \int_{-\pi/3}^{\pi/3} \frac{G(re^{i\theta})}{\tilde{G}(r)} e^{-3ni\theta} d\theta$$

As prescribed by the saddle point method, we choose

$$r = (3n + 3/4)^{2/3},$$
 (16)

so that

$$\frac{\tilde{G}(z)}{z^{3n}} = \frac{\tilde{G}(r)}{r^{3n}} e^{O((z-r)^2)}$$
(17)

(i.e., 
$$\frac{d}{dz} \log(\tilde{G}(z)z^{-3n})_{|z=r|} = 0$$
), and  
 $\theta_0 = r^{-5/8} = (3n + 3/4)^{-5/12}$ .

Observe that  $r \ge 10$  and  $0 < \theta_0 < 1/4 < \pi/3$ .

With this choice of r, we have

$$H := \frac{\sqrt{3}}{\sqrt{\pi}r^{3/4}\gamma_n} \frac{\tilde{G}(r)}{r^{3n}} = \frac{n!^2 e^{2n}}{n^{2n} 2\pi n} \frac{\sqrt{e}}{(1 + \frac{1}{4n})^{2n+1}}.$$

Stirling's formula in the form [15]  $\left|\frac{n!e^n}{n^n\sqrt{2\pi n}} - 1\right| \le s(n) = e^{\frac{1}{12n}} - 1$ , combined with the bound  $\left|\frac{\sqrt{e}}{(1+1/(4n))^{2n}} - 1\right| \le \frac{1}{16n}$ , yields

$$|H-1| \le E\left(s(n), s(n), \frac{1}{16n}, \frac{1}{4n}\right) \le \frac{1}{2n}, \qquad n \ge 11.$$
(19)

We further let

$$I_{2} = \int_{-\theta_{0}}^{\theta_{0}} \frac{G(re^{i\theta})}{\tilde{G}(r)} e^{-3ni\theta} d\theta, \qquad I_{4} = \frac{2\sqrt{\pi}}{\sqrt{3}} r^{-3/4}$$
$$I_{3} = \int_{-\theta_{0}}^{\theta_{0}} \exp\left(-\frac{3}{4}r^{3/2}\theta^{2}\right) d\theta,$$

and now aim at bounding the relative difference  $|I_1/I_4 - 1|$ . First, using (15), we have

$$\begin{aligned} |I_2 - I_1| &\leq 2 \int_{\theta_0}^{\pi/3} \frac{|G(re^{i\theta})|}{\tilde{G}(r)} d\theta \leq 4.2 \int_{\theta_0}^{\pi/3} \frac{|\tilde{G}(re^{i\theta})|}{\tilde{G}(r)} d\theta \\ &= 4.2 \int_{\theta_0}^{\pi/3} e^{\frac{2}{3}r^{3/2}(-1+\cos\frac{3\theta}{2})} d\theta \end{aligned}$$

 $|I_1 - I_2| \le 2.15r^{-9/8}$ 

and hence

Next, thanks to (17), we can write

 $\tilde{G}(re^{i\theta})e^{-3ni\theta} = \tilde{G}(r)e^{\frac{2}{3}r^{3/2}(\exp(\frac{3}{2}i\theta) - 1 - \frac{3}{2}i\theta)} = \tilde{G}(r)e^{(-\frac{3}{4}\theta^2 + u(\theta))r^{3/2}}$ 

where

Let

$$|u(\theta)| = \frac{2}{3} \left| e^{\frac{3}{2}i\theta} - 1 - \frac{3}{2}i\theta + \frac{9}{8}\theta^2 \right| \le \frac{3}{8}\theta^3.$$
(21)

$$v(\theta) = \frac{G(re^{i\theta})e^{-3in\theta}}{\tilde{G}(r)\exp(-\frac{3}{4}r^{3/2}\theta^2)} - 1.$$

Since  $\theta_0^3 r^{3/2} = r^{-3/8}$  by the choice (18), using (21) and the inequality  $|e^z - 1| \le |z|e^{|z|}$ , we have

$$e^{r^{3/2}u(\theta)} - 1| \le \frac{3}{8}r^{-3/8}e^{\frac{3}{8}r^{-3/8}} \le 0.44r^{-3/8},$$

for  $|\theta| \le \theta_0$  and  $r \ge 10$ . By (14), it follows that

$$\begin{aligned} |v(\theta)| &= \left| \frac{G(re^{i\theta})}{\tilde{G}(re^{i\theta})} e^{r^{3/2}u(\theta)} - 1 \right| \\ &\leq E(\eta_2(\theta_0)r^{-3/2}, 0.44r^{-3/8}) \leq 0.95r^{-3/8}. \end{aligned}$$

We get

$$|I_2 - I_3| = \left| \int_{-\theta_0}^{\theta_0} e^{-\frac{3}{4}r^{3/2}\theta^2} v(\theta) d\theta \right| \le 0.95r^{-3/8}I_3.$$
(22)

Finally,  $I_3$  is an incomplete Gaussian integral:

$$I_3 = \frac{2\sqrt{\pi}}{\sqrt{3}r^{3/4}} \operatorname{erf}(\frac{1}{2}\sqrt{3}r^{3/4}\theta_0) = I_4 \operatorname{erf}(\frac{1}{2}\sqrt{3}r^{1/8})$$

Lemma 2 yields

$$|I_3/I_4 - 1| \le \frac{2r^{-1/8}e^{-\frac{3}{4}r^{1/4}}}{\sqrt{3\pi}} \le 0.66r^{-1/8}e^{-\frac{3}{4}r^{1/4}}.$$
 (23)

Putting together (19, 20, 22, 23), we obtain

$$\begin{aligned} |I_1/I_4 - 1| &\leq \frac{|I_1 - I_2|}{I_4} + \left|\frac{I_2I_3}{I_3I_4} - 1\right| \\ &\leq 1.06r^{-3/8} + E(0.95r^{-3/8}, 0.66r^{-1/8}e^{-\frac{3}{4}r^{1/4}}) \\ &\leq 2.45r^{-3/8} \leq 1.9n^{-1/4}. \end{aligned}$$

It follows that

(18)

(20)

$$\left|\frac{G_n}{\gamma_n} - 1\right| = \left|H\frac{I_1}{I_4} - 1\right| \le E(0.5n^{-1}, 1.9n^{-1/4}) \le 2.4n^{-1/4}$$

for  $n \ge 11$ . It is easy to check that the final bound is valid for  $1 \le n \le 10$  as well.

Note that the above bound is not the best we can get by this method. Indeed, by choosing the exponent of r in (18) closer to -3/4, we obtain  $|G_n/\gamma_n - 1| = O(n^{-1/2} + \epsilon)$  for any  $\epsilon > 0$ . This comes at the price of a larger constant factor and thus more terms to check separately.

A first consequence of Prop. 3 is that the series G(x) has nonnegative coefficients, as stated below. We also deduce several other technical results that will be used to bound various error terms. Recall that  $c_n = n!^2G_n$ , and let  $\tau = 3/20$ .

Corollary 1: The sequence  $(c_n)$  satisfies  $0 \le c_{n+1}/c_n \le \tau$  for all  $n \ge 0$ . Accordingly, we have  $0 < G_{n+1}/G_n \le \tau (n+1)^{-2}$ . In particular, the  $G_n$  are positive.

*Proof:* Prop. 3 implies that  $c_n = (1 + \theta_n)/(4\sqrt{3}\pi 9^n)$  with  $|\theta_n| \le 2.4n^{-1/4}$ . When  $n \ge n_0 = 70000$ , we have  $|\theta_n| \le 0.148$ . This implies  $c_n \ge 0$  and  $c_{n+1}/c_n \le (1/9)(1 + \theta_{n+1})/(1 + \theta_n) \le \tau$ . The inequalities up to  $n = n_0$  are checked by computing the corresponding terms with interval arithmetic.

Corollary 2: For any  $n \ge 1$ , it holds that  $G_n \le (e/(3n))^{2n}$ .

*Proof:* With  $\theta_n$  as in Corollary 1, we have  $G_n \le \gamma_n(1+\theta_n)$ , and hence  $G_n \le 1/(9^n n!^2) \le (1/9)^n (e/n)^{2n}$ .

Lemma 4: When x > 0 and  $N + 1 \ge \sqrt{2\tau} x^{3/2}$ , we have

$$\sum_{n=0}^{N} G_n x^{3n} \le G(x) \le \sum_{n=0}^{N-1} G_n x^{3n} + 2G_N x^{3N}.$$

*Proof:* The first inequality is obvious as  $G_n \ge 0$ . To show the second one, observe that a fortiori  $\tau x^3/(n+1)^2 \le \frac{1}{2}$  for all  $n \ge N$ . Using Corollary 1, we deduce  $G_{n+1}x^3/G_n \le \frac{1}{2}$ , and hence  $\sum_{n\ge N} G_n x^{3n} \le G_N x^{3N} (1 + \frac{1}{2} + \frac{1}{4} + \cdots) = 2G_N x^{3N}$ .

Lemma 5: The function G satisfies

$$0.01e^{\frac{2}{3}x^{3/2}}x^{-3/4} \le G(x) \le 0.04e^{\frac{2}{3}x^{3/2}}x^{-3/4}$$

for all  $x \ge 1/2$ .

*Proof:* Let  $\mu(x) = E(\eta_1(0)x^{-3/2}, \sigma x^{-3/2}, \sigma x^{-3/2})$  where  $\sigma = \eta_1(\frac{2\pi}{3}) = \frac{5}{6}\sqrt{2}$ . Lemma 1 implies  $|G(x)/\tilde{G}(x) - 1| \le \mu(x)$  for  $x \ge 0$ . We can check that  $\mu(x)$  is a decreasing function and

$$0.01 \le \frac{1 - \mu(3)}{8\pi^{3/2}}, \qquad \frac{1 + \mu(3)}{8\pi^{3/2}} \le 0.04,$$

whence the desired inequality for  $x \ge 3$ . For  $0.5 < x \le 3$ , using the bounds  $0 \le e^x - (1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{1}{24}x^4) \le \frac{5}{48}x^4$  (valid for  $0 < x \le \frac{2}{3}3^{3/2}$ ) and Lemma 4, we are reduced to checking explicit polynomial inequalities.

#### IV. Roundoff error analysis

We now turn to the floating-point implementation of the functions F(x) and G(x). To make the algorithm rigorous, we will use classical techniques of error analysis that we briefly recall here. We refer the reader, e.g., to Higham [9], for proofs and complement of information.

*Notation 2:* For  $x \neq 0$ , we denote  $\text{Exp}(x) = \lfloor \log_2 |x| \rfloor + 1$ , so that  $2^{\text{Exp}(x)-1} \le |x| < 2^{\text{Exp}(x)}$ .

Notation 3: If  $x \in \mathbb{R}$ , o(x) denotes the floating-point number closest to x (ties can be decided either way). Circled operators such as  $\oplus$  denote correctly rounded floating-point operations. Floating-point numbers are represented with *t* bits of precision.

Thus, we have  $\circ(x) = x(1 + \delta)$  and  $x = \circ(x)(1 + \delta')$  with  $|\delta|, |\delta'| \le 2^{-t}$ . We will also extensively use the *relative error* counter notation  $z \langle k \rangle$ .

*Notation 4:* We write  $\widehat{z} = z \langle k \rangle$  when there exist  $\delta_1, \ldots, \delta_k$  such that  $\widehat{z} = z \prod_{i=1}^k (1 + \delta_i)^{\pm 1}$  with  $|\delta_i| \le 2^{-t}$  for all *i*.

Roughly speaking, each arithmetical operation adds one to the relative error counter of a variable. The overall error corresponding to an error counter can be bounded as follows.

*Proposition 4:* Suppose that we can write  $\hat{z} = z \langle k \rangle$  and that  $k 2^{-t} \leq 1/2$ . Then  $\hat{z} = z(1 + \theta)$  with  $|\theta| \leq 2k \cdot 2^{-t}$ .

#### V. EVALUATION OF THE MODIFIED SERIES

As we shall see in the next section, evaluating the auxiliary function F is fairly straightforward. The evaluation of G is more involved. Indeed, while  $\sum G_n x^{3n}$  is well-conditioned as a sum for  $x \ge 0$  (this is the whole point of the GMR method), the minimality of the *sequence* ( $G_n$ ) among the solutions of (12) implies that its direct recursive computation from the initial values  $G_0$  and  $G_1$  is numerically unstable (cf. [20]).

There is a standard tool to handle this situation, namely Miller's backward recurrence method [3], [20]. Miller's method

Algorithm 1: Evaluation of G **Input**: a target precision  $p \ge 1$ , a point  $x \ge 0.5$ **Output:** s such that  $|G(x) - s| \le 3 \cdot 2^{-p} G(x)$ 1 Set  $\alpha, \beta, \delta, \gamma$  s.t.  $\alpha \leq 3 e^{-1} x^{-3/2}, \beta \leq (2/3) \log_2(e) x^{3/2}$  $\gamma \gtrsim 1/\log_2(20/3), \ \delta \gtrsim (2/3) \ \log_2(e) \left((20/3)^{1/2} - 1\right) x^{3/2};$ 2  $N_0 \leftarrow \max(1, \lceil (3/10)^{1/2} x^{3/2} - 1 \rceil);$ 3 Set  $N \ge N_0$  s.t.  $\operatorname{Exp}((\alpha N)^{2N}) \ge p + 9 + \frac{3}{4} \operatorname{Exp}(x) - \lfloor \beta \rfloor$ ; 4 Set  $R \ge \max(N, \gamma (p + 2 + \delta));$ 5 Set *t* s.t.  $128(N+3)2^{-t} \le 2^{-p}$  and  $(R+2)2^{-t} \le 2^{-9}$ ; 6 for  $(a \leftarrow 1, b \leftarrow 0, i \leftarrow R-1; i \ge 0; i \leftarrow i-1)$  do  $c \leftarrow a;$ 7  $a \leftarrow (10 \otimes a) \ominus (3i+4)(3i+5) \otimes b \oslash ((i+1)(i+2));$ 8 9  $b \leftarrow c;$ if i = N - 1 then  $s \leftarrow a$ ; 10 else if i < N - 1 then  $s \leftarrow a \oplus (x^3 \otimes s \otimes (i + 1)^2)$ ; 11 12 return  $(s \otimes a) \otimes \circ (9 \Gamma(2/3)^3);$ 

allows one to accurately evaluate the minimal solution  $(c_n)$  of a recurrence of the form

 $a_2(n) u_{n+2} + a_1(n) u_{n+1} + a_0(n) u_n = 0$ ,  $a_0(n)a_2(n) \neq 0$ . (24) The idea is as follows: choose a starting index *R* and let (arbitrarily)  $u_{R+1} = 0$  and  $u_R = 1$ . Then compute  $u_n$  as

 $-a_0(n)^{-1} (a_1(n) u_{n+1} + a_2(n) u_{n+2}), \quad n = R - 1, \dots, 1, 0.$ 

It turns out that, for large *R*, the computed sequence  $(u_n)$  is close to a minimal solution of the forward recurrence. Since all minimal solutions are proportional to each other, we recover an approximation of  $c_n$  as  $c_n \approx (c_0/u_0) u_n$ .

We use Miller's method to evaluate the minimal solution  $(c_n)$  of the normalized recurrence (13), and we get an approximation of  $G(x) = \sum_{n\geq 0} G_n x^{3n}$  as  $S_N = (c_0/u_0) \sum_{n=0}^{N-1} u_n x^{3n}/(n!^2)$ . The algorithm is summed up as Algorithm 1. The rest of this section is devoted to its proof of correctness, i.e., the proof that the value *s* it returns satisfies  $|G(x) - s| \leq 3 \cdot 2^{-p}G(x)$ .

Proposition 5: With N as in Algorithm 1, the truncation error satisfies  $|\sum_{n=N}^{\infty} G_n x^{3n}| \le 2^{-p} G(x)$  for all  $x \ge 0.5$ .

*Proof:* First, because of Line 2 of the algorithm, we have  $\frac{3}{10}x^3 \le (N+1)^2$ , so that

$$\left|\sum_{n=N}^{\infty} G_n x^{3n}\right| \le 2G_N x^{3N} \le 2\left(\frac{ex^{3/2}}{3N}\right)^{2N}$$

by Lemma 4 and Corollary 2. Line 3 then ensures that

$$2\left(\frac{ex^{3/2}}{3N}\right)^{2N} \le 2\left(\alpha N\right)^{-2N} \le \frac{2^{-p}}{128} e^{\frac{2}{3}x^{3/2}} x^{-3/4} \le 2^{-p} G(x),$$

the last inequality coming from Lemma 5.

There are two sources of error besides the truncation: first,  $(u_n)$  is not exactly proportional to  $(c_n)$ , especially when *n* is close to *R*. Second, roundoff errors happen during the evaluation of  $(u_n)$ . Rigorous bounds for both sources of error have been proposed by Mattheij and van der Sluis [11]. We combine them with classical techniques (well-explained, e.g., in [5]) to choose the starting index *R* and the working precision *t* so as to to guarantee the final accuracy.

We now recall Mattheij and van der Sluis' main result (adapted to our particular case, which simplifies the statement quite a bit). Consider a recurrence of the form (24). Denote by  $(c_n)$  a minimal solution that we wish to evaluate, and let  $(d_n)$  be the solution such that  $d_0 = d_1 = 1$ . Assume that  $(d_n)$  is a dominant solution and that the sequences  $(c_n)$ ,  $(d_n)$  and  $(c_n/d_n)$  are decreasing. Define  $H = \frac{d_0}{c_0} \sum_{i=0}^{R-1} \frac{c_i}{d_i}$  and, for  $i \le R$ ,

$$U_i = \begin{pmatrix} c_i & c_i \\ c_{i+1} & c_i \frac{d_{i+1}}{d_i} \end{pmatrix} \text{ and } B_i = \begin{pmatrix} \frac{-a_1(i)}{a_0(i)} & \frac{-a_2(i)}{a_0(i)} \\ 1 & 0 \end{pmatrix}.$$

Let  $v_R \in \mathbb{R}^2$  be a column vector, and for  $i \leq R-1$ , let  $v_i$  be the result of the floating-point evaluation of  $B_i v_{i+1}$  at precision *t*. Write  $v_i = (u_i, u_{i+1})^T$ . If all operations were exact,  $(u_i)$  would be the solution of the recurrence such that  $(u_R, u_{R+1})^T = v_R$ . To take rounding errors into account, we write  $v_i = (B_i + 2^{-t}G_i)v_{i+1}$  for some matrix  $G_i$  instead. Define  $y_R = (y_{R1}, y_{R2})^T = U_R^{-1}v_R$ . Let  $\mathcal{F}_i = ||U_i^{-1}G_iU_{i+1}||$ , the matrix norm being subordinate to the  $|| \cdot ||_{\infty}$  norm for vectors, and let  $\mathcal{F} \ge \max_i \mathcal{F}_i$ .

Theorem 1: [11, Theorem 4.1] Provided that the quantities

$$\mathcal{F}R2^{-t}, \quad \frac{c_R d_0}{d_R c_0} \frac{y_{R2}}{y_{R1}}, \quad \frac{||y_R||_{\infty}}{|y_{R1}|} (R+H)(1.3\mathcal{F}2^{-t})$$

are all bounded by 0.1, the approximate value  $u_i$  computed by Miller's algorithm satisfies  $(c_0/u_0) u_i = c_i (1 + \theta_i)$  for some  $\theta_i$  such that  $|\theta_i| \le T_i + R_i$ , where

$$T_{i} = 1.5 \left( \frac{c_{R} d_{i}}{c_{i} d_{R}} + \frac{c_{R} d_{0}}{c_{0} d_{R}} \right) \left| \frac{y_{R2}}{y_{R1}} \right|, \quad R_{i} = 1.5 \frac{\|y_{R}\|_{\infty}}{y_{R1}} \varepsilon (i + 2H).$$

and  $\varepsilon = 1.3\mathcal{F}2^{-t}$ .

Turning back to the special case  $c_n = n!^2G_n$ , Theorem 1 applied to (13) yields the following. Recall that  $\tau = 3/20$ .

Corollary 3: Set  $v_R = (1, 0)^T$  and

$$B_i = \begin{pmatrix} 10 & -r(i) \\ 1 & 0 \end{pmatrix} \text{ where } r(n) = \frac{(3n+4)(3n+5)}{(n+1)(n+2)}$$

Then, in the notation of Theorem 1, we have  $T_i \le \tau^{R-i}$  and  $R_i \le 76.5(i+4)2^{-t} \le 76.5(N+3)2^{-t}$  for all i < N.

Proving this corollary still requires some work. We postpone it for a bit to explore the consequences of this statement.

Observe that lines 8 and 9 of Algorithm 1 are equivalent to a floating-point evaluation of  $B_i v_{i+1}$  where  $v_{i+1} = (a, b)^{T}$ . Hence, at each loop turn, we have  $a = u_i$  just after line 8. Lines 10 and 11 are a Horner-like evaluation scheme, so that  $s \approx \sum_{i=0}^{N-1} u_i x^{3i} / i!^2$  at the end of the loop. More precisely, assuming  $x^3$  is approximated by  $\circ(x) \otimes \circ(x) \otimes \circ(x)$  and division by  $(i + 1)^2$  is performed as two successive divisions by (i + 1), an easy induction shows that one can write

$$s = \sum_{i=0}^{N-1} \left( u_i \frac{x^{3i}}{i!^2} \right) \langle 9(i+1) \rangle \,.$$

Line 12 adds 3 to all error counters. Using Prop. 4 we conclude that, at the end of the algorithm, we have

$$s = \sum_{i=0}^{N-1} \frac{c_0 \, u_i}{u_0} \cdot \frac{x^{3i}}{i!^2} \, (1+\mu_i) = \sum_{i=0}^{N-1} G_i \, x^{3i} (1+\mu_i) (1+\theta_i),$$

where  $|\mu_i| \le 2 (9(i+1)+3) \cdot 2^{-t} \le 18(N+3) 2^{-t}$  and  $|\theta_i| \le T_i + R_i$ .

Since  $R \ge N$ , we have  $T_i \le \tau$  for all i < N. The definition of *t* implies  $128(N+3)2^{-t} \le 2^{-p} \le 1/2$ , hence  $R_i \le 76.5/256$ .

Altogether, this ensures that  $|\theta_i| \le 1$ . So, writing  $(1+\mu_i)(1+\theta_i) = 1 + \delta_i$ , we have

$$|\delta_i| \le 2|\mu_i| + |\theta_i| \le 112.5(N+3)2^{-t} + \tau^{R-i} \le 2^{-p} + \tau^{R-i},$$

and therefore  $\left|s - \sum_{i=0}^{N-1} G_i x^{3i}\right| \le 2^{-p} G(x) + \tau^R G(\tau^{-1/3} x)$ . Lemma 6: For x > 0.5, we have  $\tau^R G(\tau^{-1/3} x) \le 2^{-p} G(x)$ . Proof: It follows from Lemma 5 (and  $\tau < 1$ ) that

$$\frac{G(x)}{G(\tau^{-1/3}x)} \ge \frac{1}{4} \exp\left(\frac{2}{3}x^{3/2}(1-\tau^{-1/2})\right),$$

and the algorithm ensures that

$$R \ge \frac{1}{\log_2 \tau^{-1}} \left( p + 2 + \frac{2}{3} \log_2(e)(\tau^{-1/2} - 1) x^{3/2} \right),$$

whence  $\tau^R \leq \frac{1}{4} 2^{-p} \exp(\frac{2}{3} x^{3/2} (1 - \tau^{-1/2}))$  and the result. Since  $|G(x) - s| \leq |G(x) - \sum_{i=0}^{N-1} G_i x^{3i}| + |s - \sum_{i=0}^{N-1} G_i x^{3i}|$ , the correctness of Algorithm 1 is a consequence of Prop. 5 and

correctness of Algorithm 1 is a consequence of Prop. 5 and the above discussion.

*Theorem 2:* The value *s* returned by Algorithm 1 satisfies  $|G(x) - s| \le 3 \cdot 2^{-p}G(x)$ .

The remainder of this section is devoted to the proof of Corollary 3. We begin with a crucial lemma. Let  $(d_n)$  be the solution of (13) defined by  $d_0 = d_1 = 1$ .

Lemma 7: For all  $n \ge 1$ , we have  $d_{n+1} \le d_n \le (1+\eta(n)) d_{n+1}$ with  $\eta(n) = 1/(3n^2)$ .

*Proof:* We proceed by induction. Since  $d_2 = 9/10$ , the property is true for n = 1. Now, supposing it for an arbitrary n, we get  $(9 - \eta(n))d_{n+1} \le 10d_{n+1} - d_n \le 9d_{n+1}$ , so

$$\frac{9-\eta(n)}{r(n)}d_{n+1} \le d_{n+2} \le \frac{9}{r(n)}d_{n+1}, \quad r(n) = \frac{(3n+4)(3n+5)}{(n+1)(n+2)}.$$

We conclude by observing that  $9/r(n) \le 1$  and  $r(n)/(9-\eta(n)) \le 1 + \eta(n+1)$  for  $n \ge 1$ .

Corollary 4: For all *n*, we have  $0.783 \le d_n \le 1$ .

*Proof:* By Lemma 7,  $(d_n)$  is decreasing and  $d_0 = 1$ : this proves the right-hand side. For  $n \ge 100$ , Lemma 7 implies

$$d_{100} \le d_n \prod_{i=100}^{n-1} (1+\eta(i)) \le d_n \frac{p_{\infty}}{p_{99}}, \quad p_k = \prod_{i=1}^k (1+\eta_i).$$

Using the exact value  $p_{\infty} = \frac{\sqrt{3}}{\pi} \sinh(\frac{\pi}{\sqrt{3}})$  [1, Eq. 4.36.1], we check that  $d_n \ge d_{100} p_{99} p_{\infty}^{-1} \ge 0.783$  for  $n \ge 100$ . As  $(d_n)$  is decreasing, the inequality holds for n < 100 too.

This estimate, combined with Corollary 1 gives almost all we need to check the hypotheses of Theorem 1. We use the notation introduced for the statement of Theorem 1.

*Corollary 5:* The sequences  $(c_n)$ ,  $(d_n)$  and  $(c_n/d_n)$  are decreasing. Moreover, the following inequalities hold:  $H \le 2$ ,  $|y_{R2}/y_{R1}| \le \frac{1}{6}$ ,  $||y_R||_{\infty}/|y_{R1}| = 1$ , and det  $U_i \ge \frac{3}{4}c_i^2$ .

*Proof:* Corollary 1 shows that  $(c_n)$  is decreasing and Lemma 7 shows that  $(d_n)$  is decreasing. Together, they imply  $\frac{c_{n+1}}{d_{n+1}}/\frac{c_n}{d_n} \le \tau (1 + 1/3n^2) \le \frac{1}{5}$  for  $n \ge 1$ , and we can check that  $c_1/d_1 \le c_0/d_0$ . Hence  $(c_n/d_n)$  is decreasing.

Corollary 1 also implies  $c_n \le \tau^n c_0$  for any *n*, and Corollary 4 shows that  $d_0 \le d_n/0.783$  for any *n*. It follows that

$$H = \frac{d_0}{c_0} \sum_{i=0}^{R-1} \frac{c_i}{d_i} \le \frac{1}{0.783} \sum_{i=0}^{R-1} \tau^i \le 2.$$

We have  $d_0/d_1 = 1$ ,  $d_1/d_2 = 10/9$ , and  $d_i/d_{i+1} \le 1 + 1/(3i^2) \le 1$ 10/9 for  $i \ge 2$ , and, by definition of  $U_R$  and  $v_R$ ,

$$y_{R} = U_{R}^{-1} v_{R} = \frac{c_{R}}{\det U_{R}} \begin{pmatrix} d_{R+1}/d_{R} & -1 \\ -c_{R+1}/c_{R} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{c_{R}}{\det U_{R}} \begin{pmatrix} d_{R+1}/d_{R} \\ -c_{R+1}/c_{R} \end{pmatrix}$$

It follows that  $|y_{R2}/y_{R1}| \le \frac{10}{9}\tau = \frac{1}{6}$ . This implies  $|y_{R2}| \le |y_{R1}|$ , and therefore  $||y_R||_{\infty}/|y_{R1}| = 1$ .

Finally, from the expression det  $U_i = c_i^2 (d_{i+1}/d_i - c_{i+1}/c_i)$ , we obtain  $c_i^{-2} \det U_i \ge (\frac{9}{10} - \tau) = \frac{3}{4}$ . Lemma 8: A suitable value for  $\mathcal{F}$  is 39.

*Proof:* The multiplication  $B_i v_i$  is performed on lines 8 and 9. Denoting by a' and b' the new values of a and b, we can write b' = a and, with r(i) as in Corollary 3,

$$a' = 10a\langle 2 \rangle - r(i)b\langle 5 \rangle = a' = 10a(1+\theta) - r(i)b(1+\theta')$$

where  $|\theta| \le 4 \cdot 2^{-t}$  and  $|\theta'| \le 10 \cdot 2^{-t}$  by Prop. 4. (This assumes that the multiplication by r(i) is performed through four successive multiplications and divisions). Therefore, we have

$$|\mathcal{G}_i| \le \begin{pmatrix} 10 \cdot 4 & 10r(i) \\ 0 & 0 \end{pmatrix}$$

where, for matrices,  $|A| \leq |B|$  means that the inequality holds entrywise. Since moreover

$$|U_i^{-1}| \le \frac{|c_i|}{|\det U_i|} \begin{pmatrix} d_{i+1}/d_i & 1\\ c_{i+1}/c_i & 1 \end{pmatrix} \le \frac{4}{3c_i} \begin{pmatrix} 1 & 1\\ 3/20 & 1 \end{pmatrix},$$
$$|U_{i+1}| \le c_{i+1} \begin{pmatrix} 1 & 1\\ c_{i+2}/c_{i+1} & d_{i+2}/d_{i+1} \end{pmatrix} \le c_{i+1} \begin{pmatrix} 1 & 1\\ 3/20 & 1 \end{pmatrix},$$

and  $\mathcal{F}_i \leq |U_i^{-1}| \cdot |\mathcal{G}_i| \cdot |U_{i+1}|$ , we get

$$\mathcal{F}_{i} \leq \frac{4}{3} \cdot \frac{3}{20} \begin{pmatrix} 40 + \frac{3}{2}r(i) & 40 + 10r(i) \\ \frac{3}{20}(40 + \frac{3}{2}r(i)) & \frac{3}{20}(40 + 10r(i)) \end{pmatrix}.$$

Hence  $\|\mathcal{F}_i\| \le 8 + \frac{3}{10} r(i) + 8 + 2 r(i)$ . The result follows because  $r(i) \leq 10$  for all  $i \geq 0$ .

We can finally prove Corollary 3.

Proof: In order to apply Theorem 1, we need to check that (i)  $39 R2^{-t} \le 0.1$ , (ii)  $\frac{c_R d_0}{d_R c_0} \le 0.1 \frac{y_{R1}}{y_{R2}}$ , and (iii)  $(R+2)(50.7 \cdot 2^{-t}) \le 0.1$ . By definition of t,  $R + 2 \le 2^{t-9}$ , so (iii) is satisfied. We notice that (iii) trivially implies (i). Finally, by Corollary 5, it suffices to prove  $\frac{c_R d_0}{d_R c_0} \le 0.6$  to prove (ii). This is clearly true since  $d_0/d_R \le 1/0.783$  and  $c_R/c_0 \le \tau^R \le \tau^N \le \tau$ .

In conclusion, we can apply Theorem 1, hence

$$T_{i} = 1.5 \left( \frac{c_{R} d_{i}}{c_{i} d_{R}} + \frac{c_{R} d_{0}}{c_{0} d_{R}} \right) \left| \frac{y_{R2}}{y_{R1}} \right| \le \frac{1.5}{0.783} \left( \tau^{R-i} + \tau^{R} \right) \frac{1}{6}.$$

Therefore,  $T_i \leq 0.639 \cdot \tau^{R-i} \leq \tau^{R-i}$  as announced. Theorem 1 together with Corollary 5 give  $R_i = 1.5 (50.7 \cdot 2^{-t})(i + 2H) \leq$  $76.5 \cdot (i+4) 2^t$ .

#### VI. EVALUATION OF THE AUXILIARY SERIES

The implementation of the auxiliary series F is much easier than that of G: the recurrence is a simple two-term recurrence that can be accurately evaluated by forward recursion. We limit ourselves to a sketch of the (fairly standard) algorithm.

A variable  $a_0$  is used to successively evaluate  $F_0$ ,  $F_3x^3$ ,  $F_6x^6$ , etc., using the recurrence (1). Accordingly, two variables  $a_1$ and  $a_2$  are used to evaluate the successive values of  $F_{3n+1}x^{3n+1}$ and  $F_{3n+2}x^{3n+2}$ . Each step adds 10 to the relative error counter of each variable. A variable s is used to accumulate the sum

as the variables  $a_k$  are updated. Therefore, after step K, we can write  $s = \sum_{i=0}^{3K-1} F_i x^i \langle 1 + 10(i/3) + 3K \rangle$ , or, bounding all errors uniformly

$$s = \sum_{i=0}^{N-1} F_i x^i \left\langle 5(N+1) \right\rangle, \qquad N = 3K.$$

It is easy to see that q(n) = 2(2n+1)/((n+1)(n+2)(n+3))decreases for  $n \ge 1$ , hence the loop can be stopped as soon as (i)  $q(n)x^3 < 1/2$ , and (ii)  $a_0, a_1, a_2 < 2^{\text{Exp}(s)-p-4}$ . These conditions ensure that the remainder of the series is bounded by  $(a_0 + a_1 + a_2) < \frac{3}{16} 2^{-p} 2^{\text{Exp}(s)}$ .

It is clear from Prop. (1) that  $F_{n+3} \leq 4F_n/n^2$  for any n, hence (using  $n! \approx (n/e)^n$ ) we have  $F_n \approx (4e^2/n^2)^{n/3}$ . This is most likely an overestimation of the true value. Moreover, we can approximate F(x) by  $\frac{1}{32}x^{-1/2} \exp(\frac{4}{3}x^{3/2})$  for x > 0.5 and by  $2^{-3} + 2^{-4}x$  for  $0 < x \le 0.5$ . These estimates are used to get a rough overestimation N of the necessary truncation rank. Based on this estimation the working precision t is chosen so that  $10(N+1)2^{1-t} \le 2^{-3-p}$ . Hence, we have  $|\sum_{i=0}^{N-1} F_i x^i - s| \le 2^{-3-p} s \le 2^{\operatorname{Exp}(s)-3-p}$ .

The initial estimation of the truncation rank is very unlikely to be underestimated. In the case it would be smaller than the actual truncation rank decided on-the-fly by the above criterion, this is checked a posteriori and, if necessary, the evaluation is run again with an updated working precision.

We conclude by writing  $|F(x) - \bar{s}| \le |F(x) - \sum_{i=0}^{N-1} F_i x^i| + |s - \sum_{i=0}^{N-1} F_i x^i| \le \frac{8}{16} 2^{-p} 2^{\text{Exp}(s)} \le 2^{-p} s.$ 

#### VII. COMPLETE ALGORITHM

Assume  $p \ge 3$ . From the previous sections, it appears that we computed  $\widehat{G}$  such that  $\widehat{G} = G(x)(1+\theta_1)$  with  $|\theta_1| \le 3 \cdot 2^{-p}$ , and we computed  $\widehat{F}$  such that  $F(x) = \widehat{F}(1 + \theta_2)$  with  $|\theta_2| \le 2^{-p}$ . Hence  $\widehat{G}/\widehat{F} = (G(x)/F(x))(1+\theta_3)$  where  $|\theta_3| = |\theta_1+\theta_2(1+\theta_1)| \le 5 \cdot 2^{-p}$ . Indeed, the division is performed in floating-point arithmetic at precision p, leading a final result  $\widehat{A} = (\widehat{G}/\widehat{F})(1 + \theta_4)$  with  $|\theta_4| \leq 2^{-p}$ . Hence, finally,  $A = \operatorname{Ai}(x)(1+\theta_5)$  with  $|\theta_5| = |\theta_3 + \theta_5|$  $|\theta_4(1+\theta_3)| \le 7 \cdot 2^{-p} \le 2^{-(p-3)}.$ 

We developed a prototype implementation of this algorithm, based on the multiple precision floating-point library MPFR [7]. In order to test the implementation, we compared the results with that of the built-in implementation of Ai(x) available in MPFR, run with a larger precision. Random tests using several thousands of points x and target precisions p yield relative errors smaller than  $2^{-(p-3)}$  between the result of our implementation and the result of MPFR, as predicted by theory.

We also ran our implementation and MPFR with the same accuracy, in order to compare the performance of both implementations. The result is shown on Figure 3 (MPFR 3.1.1, GMP 4.3.1, on an Intel Xeon at 2.67GHz). Our method is faster than MPFR when x is fairly large. This is all the benefit of reducing the cancellation: when x is large, the working precision of MPFR has a large overhead because of the bad condition number of the series. In contrast, our method keeps a reasonable precision, of the same order of magnitude as the target precision. Both implementations are comparable for small values x and target precisions; and MPFR wins over our

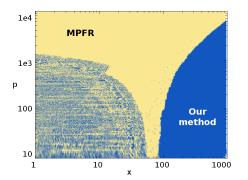


Figure 3. Fastest method as a function of x and p (scales are logarithmic).

implementation only for intermediate values of x and fairly large precisions, when our implementation pays the cost of evaluating two series instead of a single one, with little benefit in terms of working precision.

#### VIII. OUTLOOK: TOWARDS A GMR algorithm?

As mentioned in the introduction, we see the present work as a case study. Indeed, in spite of the many technical details that occupy much of the space of this article, we really used very few specific properties of the Airy function besides Equation (3). Looking back, our analysis essentially relies on the following ingredients.

(i) *The ability to find auxiliary series*. The indicator functions used in the GMR method depend only on the behaviour at (complex) infinity of the entire functions they are associated to. In the case of the solution of a LODE with analytic coefficients, this behaviour is entirely determined by the differential equation along with a finite number of "asymptotic initial values" [19], [18]. Once the indicator function is known, it remains to exhibit appropriate auxiliary series. Doing this in a truly general way remains an open problem. Yet, both the original GMR method and our variant apply to many cases, and it is likely that they can be combined and further generalized.

(ii) An efficient way to compute their coefficients. This seems to be considered a major limitation in the original GMR paper [8]. But, as already mentioned, recurrences with polynomial coefficients automatically exist as soon as both the original function to evaluate and the auxiliary series satisfy differential equations with polynomial coefficients. Numerical stability is not much of an issue in the case of three-term recurrences, thanks to Miller's method, though many technical details must be settled. The situation is more complicated in general for recurrences of higher order. Observe, though, that we proved the minimality of  $(G_n)$  by using essentially the same asymptotic properties that were exploited by the GMR method in the first place. The minimality may hence not be fortuitous and might generalize.

(iii) Upper and lower bounds on the coefficients and sums of the series F and G. All these bounds were derived, in a pretty systematic way, from the asymptotic expansion of Ai at infinity completed with Lemma 1. Bounds similar to that from Lemma 1 can themselves often be obtained from a LODE [13].

(iv) *Roundoff error analyses*. Our error analyses follow a very regular pattern and could probably be abstracted to a more

general case or automated.

In short, most steps of our study could apparently be performed in a systematic, if not *algorithmic*, way starting from Eq. (3) plus a moderate amount of additional information. Systematizing the GMR method based on this observation seems a promising line of research. Solutions of LODE with polynomial coefficients are known in Computer Algebra as *D*-*finite*, or *holonomic*, functions. Powerful symbolic algorithms are available to work with this class of functions, and already cover points (i)–(iii) above to some extent [2]. It is perhaps too ambitious, though, to aim to handle the whole class of D-finite entire functions. Thus, at this point, we suggest looking for a natural subclass to which the method applies in a truly systematic way, hopefully to the point that it can be *automated* using Computer Algebra.

Acknowledgments: We thank Paul Zimmermann for pointing out the GMR article to us.

#### References

- [1] *Digital library of mathematical functions*, 2010, Online companion to [12], http://dlmf.nist.gov/.
- [2] A. Benoit, F. Chyzak, A. Darrasse, S. Gerhold, M. Mezzarobba, and B. Salvy, *The dynamic dictionary of mathematical functions (DDMF)*, ICMS 2010 (K. Fukuda, J. van der Hoeven, M. Joswig, and N. Takayama, eds.), LNCS, vol. 6327, Springer, 2010, pp. 35–41.
- [3] W. G. Bickley, L. J. Comrie, J. C. P. Miller, D. H. Sadler, and A. J. Thompson, *Bessel functions*, Mathematical Tables, vol. X, British Association for the Advancement of Science, 1952.
- [4] R. P. Brent and P. Zimmermann, *Modern computer arithmetic*, Cambridge University Press, 2010.
- [5] S. Chevillard, The functions erf and erfc computed with arbitrary precision and explicit error bounds, Information and Computation 216 (2012), 72 – 95.
- [6] P. Flajolet and R. Sedgewick, Analytic combinatorics, Cambridge University Press, 2009.
- [7] L. Fousse, G. Hanrot, V. Lefèvre, P. Pélissier, and P. Zimmermann, MPFR: A multiple-precision binary floating-point library with correct rounding, ACM TOMS 33 (2007), no. 2, 13:1–13:15.
- [8] W. Gawronski, J. Müller, and M. Reinhard, *Reduced cancellation in the evaluation of entire functions and applications to the error function*, SIAM Journal on Numerical Analysis 45 (2007), no. 6, 2564–2576.
- [9] N. J. Higham, Accuracy and Stability of Numerical Algorithms, second ed., SIAM, 2002.
- [10] B. Y. Levin, Lectures on entire functions, AMS, 1996.
- [11] R. M. M. Mattheij and A. van der Sluis, Error Estimates for Miller's Algorithm, Numerische Mathematik 26 (1976), 61–78.
- [12] F. W. Olver, D. W. Lozier, R. F. Boisvert, and C.W. Clark (eds.), NIST handbook of mathematical functions, Cambridge University Press, 2010.
- [13] F. W. J. Olver, Asymptotics and special functions, A K Peters, 1997.
- [14] M. Reinhard, Reduced cancellation in the evaluation of entire functions and applications to certain special functions, Ph.D. thesis, Universität Trier, 2008.
- [15] H. Robbins, A remark on Stirling's formula, The American Mathematical Monthly 62 (1955), no. 1, 26–29.
- [16] R. P. Stanley, *Enumerative combinatorics*, vol. 2, Cambridge University Press, 1999.
- [17] I. A. Stegun and R. Zucker, Automatic computing methods for special functions, Journal of Research of the National Bureau of Standards 74B (1970), 211–224.
- [18] M. van der Put and M. F. Singer, *Galois theory of linear differential equations*, Springer, 2003.
- [19] W. R. Wasow, Asymptotic expansions for ordinary differential equations, Wiley, 1965.
- [20] J. Wimp, Computation with recurrence relations, Pitman, Boston, 1984.