Evaluation of Ai(x) with Reduced Cancellation

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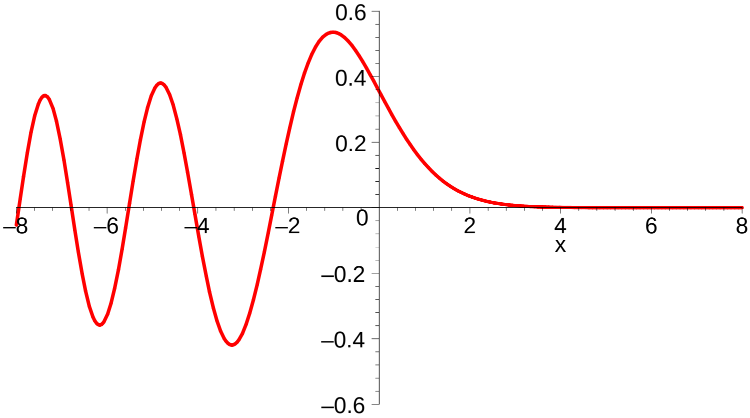
The Airy Function $\mathrm{Ai}(x)$



$$\mathbf{Ai''(x) = x\,Ai(x)} \qquad \mathrm{Ai}(0) = \frac{1}{3^{2/3}\,\Gamma(2/3)} \qquad \mathrm{Ai}'(0) = -\frac{1}{3^{1/3}\,\Gamma(1/3)}$$

Multiple-Precision Evaluation for $x > 0$

Standard Approach

"Small" x: Taylor Series at 0

- catastrophic cancellation for moderately large x
- need $p_{\text{work}} \gg p_{\text{res}}$

for $n = 0, 1, \ldots, N-1$

$$t_n := a_1(n) \cdot t_{n-1} \cdot x + a_2(n) \cdot t_{n-1}\, x^2 + \cdots + a_k(n) \cdot t_{n-k} \cdot x^k$$

$$s := s + t_n$$

(floating-point, precision p_{work})

"Large" x: Asymptotic Expansion at ∞

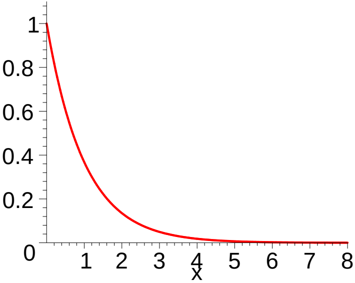
This talk

New evaluation algorithm for "small" x with $p_{\text{work}} \approx p_{\text{res}}$

Complete error analysis

Cancellation?

A Simple Example



$$\exp(-x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} x^n$$

$x = 20$

```
> x := 20:

> add((-20.)^n/n!, n=0..99);
```

$$-.12115250e-1$$

```
> exp(-20.);
```

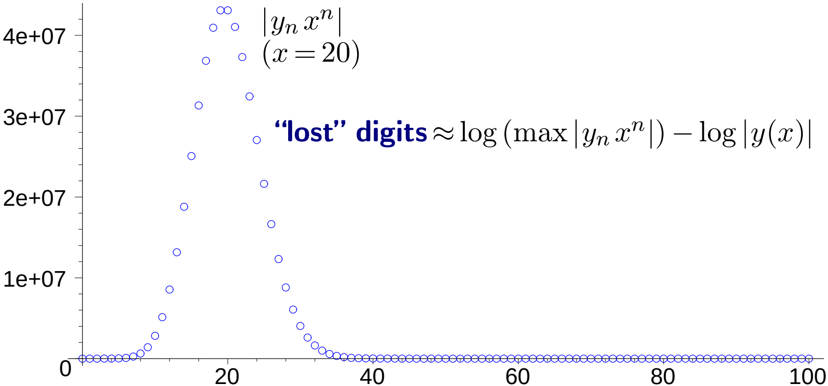
$$.2061153622e-8$$

```
> Digits := 30;
  add((-20.)^n/n!, n=0..99);
```

$$\mathbf{Digits} := 30$$

$$.206115362243865948417e-8$$

Catastrophic Cancellation

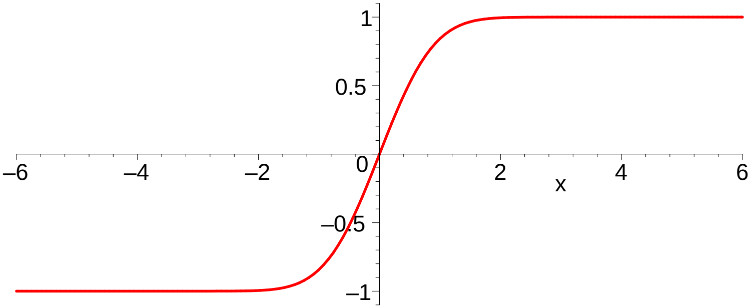


Except that...

$$\exp(-x) = \frac{1}{\exp(x)}$$

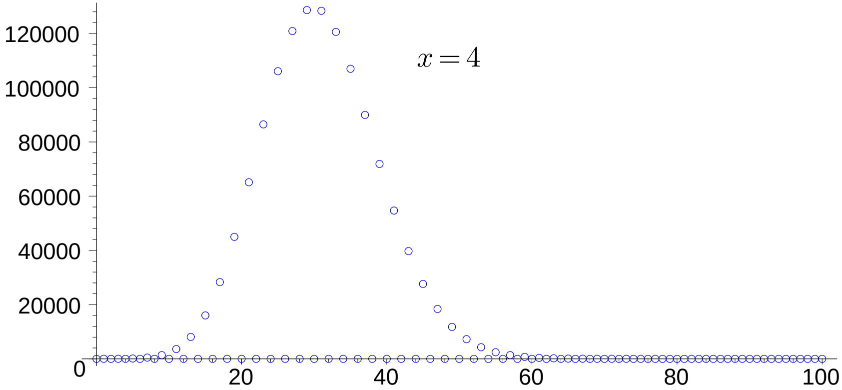
Another Example

The Error Function



$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\left(x - \frac{1}{3}x^3 + \frac{1}{10}x^5 - \frac{1}{42}x^7 + \frac{1}{216}x^9 - \cdots\right)$$

The Error Function



catastrophic cancellation

But...

Series Expansions

7.1.5 $$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{n!(2n+1)}$$

7.1.6 $$= \frac{2}{\sqrt{\pi}} e^{-z^2} \sum_{n=0}^{\infty} \frac{2^n}{1 \cdot 3 \ldots (2n+1)} z^{2n+1}$$

[Abramowitz & Stegun 1972, p. 297]

Algorithm

1. Compute $\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{2^n x^{2n+1}}{1 \cdot 3 \cdots (2n+1)}$ positive terms, no cancellation
2. Compute $\exp(x^2)$
3. Divide

Where

does this formula

“come from”?

The Gawronski-Müller-Reinhard Method

Or: How Complex Analysis "explains" the previous trick

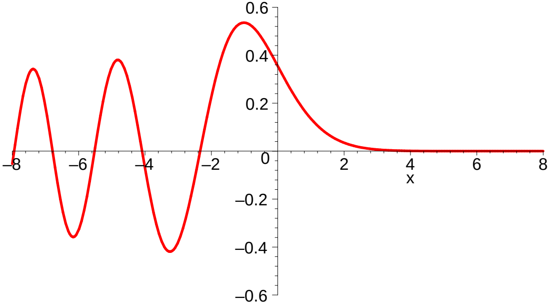
Idea: **Find F and G** such that

1. $y(x) = \dfrac{G(x)}{F(x)}$
2. F and G computable with little cancellation

W. Gawronski, J. Müller, M. Reinhard. *SIAM J. Num. An.*, 2007

M. Reinhard. Phd thesis, Universität Trier, 2008

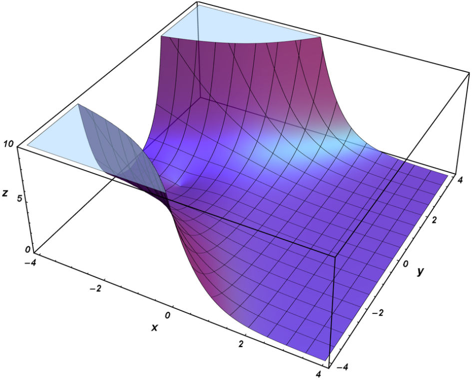
Back to Ai



$$\mathrm{Ai}(x) = A - B\,x + \frac{A}{6}\,x^3 - \frac{B}{12}\,x^4 + \frac{A}{180}\,x^6 - \frac{B}{504}\,x^7 + \frac{A}{12960}x^9 - \cdots$$

$$= A\sum_{n=0}^{\infty} \frac{1\cdot 4\cdots(3\,n-2)}{(3\,n)!}\,x^{3n} - B\sum_{n=0}^{\infty} \frac{2\cdot 5\cdots(3\,n-1)}{(3\,n+1)!}\,x^{3n+1}$$

Asymptotics



$$\mathrm{Ai}(z) \sim \frac{\exp\left(-\frac{2}{3}\,z^{3/2}\right)}{2\,\sqrt{\pi}\,z^{1/4}}$$

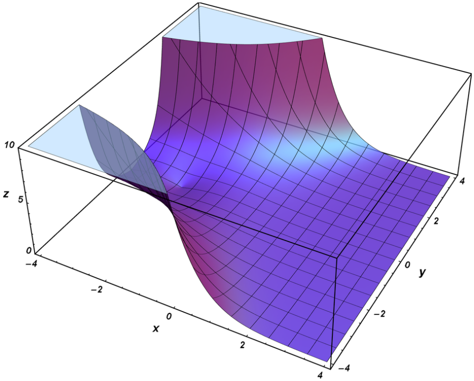
as $z \to \infty$

in any sector

$\{z \in \mathbb{C} | -\varphi < \arg z < \varphi\}$

with $\varphi < \pi$

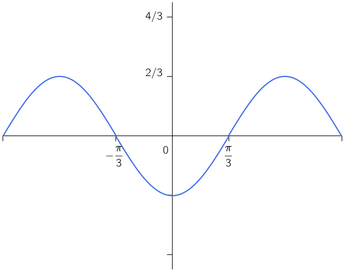
Asymptotics



$$\mathrm{Ai}(z) \sim \frac{\exp\left(-\frac{2}{3}\,z^{3/2}\right)}{2\sqrt{\pi}\,z^{1/4}}$$

Order $\rho = 3/2$

Indicator $h(\theta) = -\frac{2}{3}\cos\frac{3\,\theta}{2}$



$$|\mathrm{Ai}(r\,e^{i\theta})| \approx \exp\left(\boldsymbol{h}(\theta)\,r^{\boldsymbol{\rho}}\right)$$

for large r

Lost in Cancellation

$|y(r\,e^{i\theta})| \approx \exp\left(\boldsymbol{h}(\theta)\, r^{\boldsymbol{\rho}}\right)$

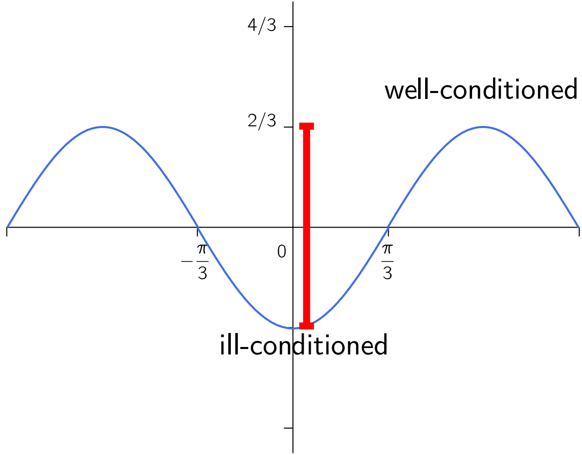
for large r

$\max_n |y_n\, z^n| = M(|z|)^{1+o(1)}$

$M(r) = \max_{|z|=r} |y(z)|$

$$\begin{aligned}
\textbf{“lost” digits} \;&\approx\; \log_{10}\Bigl(\max_n |y_n\, z^n|\Bigr) - \log_{10}|y(z)| \\
&\approx\; \log_{10} M(|z|) - \log_{10}|y(z)| \\
&\approx\; \bigl(r^{\rho} \max_{\varphi} h(\varphi)\bigr) - r^{\rho}\, h(\theta) \qquad (z = r\,e^{i\theta}) \\
&=\; r^{\rho}\,(\boldsymbol{\max h - h(\theta)})
\end{aligned}$$

Lost in Cancellation



$$\textbf{lost digits} \approx r^{\rho}\,(\max h - h(\theta))$$

The GMR Method

$$\begin{cases} |F(z)| \approx \exp\left(\boldsymbol{h_F(\theta)}\, r^\rho\right) \\ |G(z)| \approx \exp\left(\boldsymbol{h_G(\theta)}\, r^\rho\right) \end{cases} \quad \Rightarrow \quad \left|\frac{G(z)}{F(z)}\right| \approx \exp\Big[\underbrace{\left(\boldsymbol{h_G(\theta)} - \boldsymbol{h_F(\theta)}\right)}_{h_{G/F}(\theta)} r^\rho\Big]$$

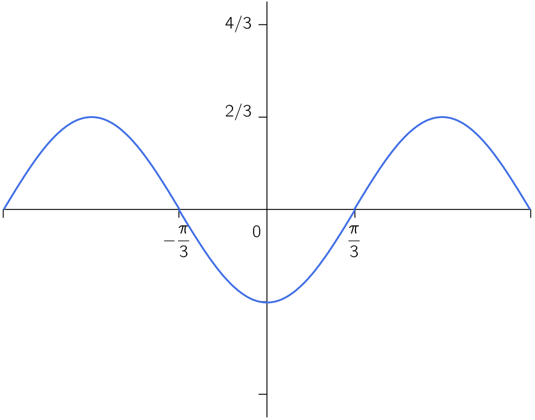
Idea (refined): look for

- an auxiliary series F,
- a modified series $G = y\,F$,

both of order ρ,

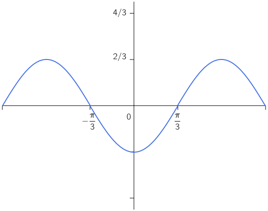
such that h_F and $h_G \approx$ their max for $\theta = 0$

Auxiliary Series: A First Try

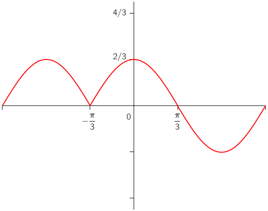


$$\mathrm{Ai}(x) = \frac{G(x)}{\exp\left(\alpha\, x^{\mathbf{3/2}}\right)}?$$

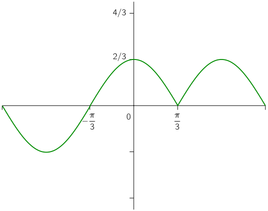
Indicators



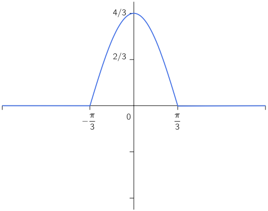
$\mathrm{Ai}(x)$



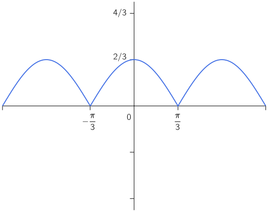
$\mathrm{Ai}(j^{-1}\,x)$



$\mathrm{Ai}(j\,x)$



$\boldsymbol{F(x)} = \mathrm{Ai}(j\,x)\,\mathrm{Ai}(j^{-1}\,x)$



$\boldsymbol{G(x)} = \mathrm{Ai}(x)\,\mathrm{Ai}(j\,x)\,\mathrm{Ai}(j^{-1}\,x)$

How do we

evaluate

the auxiliary series?

Computer Algebra to the Rescue

A function y is **D-finite** (holonomic) when it satisfies a linear ODE with polynomial coefficients.

Examples: $\mathbf{Ai}(\boldsymbol{x}), \exp(x), \mathrm{erf}(x)\ldots$ $\qquad \mathrm{Ai}''(x) = x\,\mathrm{Ai}(x)$

If $f(x)$, $g(x)$ are D-finite, then:

- $f(x) + g(x)$ and $f(x) \cdot g(x)$ too

  $F(x) = \mathrm{Ai}(j\,x) \cdot \mathrm{Ai}(j^{-1}\,x)$ $\qquad F'''(x) = 4\,x\,F'(x) + 2\,F(x)$

- The Taylor coefficients of $f(x)$ obey a linear recurrence relation with polynomial coefficients

  $F(x) = \sum_{n=0}^{\infty} F_n\,x^n$ $\qquad F_{n+3} = \frac{2\,(2\,n+1)}{(n+1)\,(n+2)\,(n+3)}\,F_n$

The Auxiliary Series $F(x)$

$$F(x) = \mathrm{Ai}(j\,x)\,\mathrm{Ai}(j^{-1}\,x) = \sum_{n=0}^{\infty} F_n\,x^n$$

D-Finiteness

$$\boldsymbol{F_{n+3}} = \frac{2\,(2\,n+1)}{(n+1)\,(n+2)\,(n+3)}\,\boldsymbol{F_n}$$

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

Two-term recurrence ➡ Easy to evaluate

Obviously $F_n > 0$ ➡ No cancellation

The Modified Series $G(x)$

$$G(x) = \mathrm{Ai}(x)\, F(x) = \sum_{n=0}^{\infty} G_n\, \boldsymbol{x^{3n}}$$

D-Finiteness

$$\boldsymbol{G_{n+2}} = \frac{10\,(n+1)^2\, \boldsymbol{G_{n+1}} - \boldsymbol{G_n}}{(n+1)\,(n+2)\,(3\,n+4)\,(3\,n+5)}$$

$$G_0 = \frac{1}{9\,\Gamma\left(\frac{2}{3}\right)^3} \qquad G_1 = \frac{1}{18\Gamma\left(\frac{2}{3}\right)^3} - \frac{1}{3\,\Gamma\left(\frac{1}{3}\right)^3}$$

$$G(x) = 0.44749 \cdot 10^{-1} + 0.50371 \cdot 10^{-2}\, x^3 + 0.14053 \cdot 10^{-3}\, x^6 + 0.17388\, 10^{-5}\, x^9 + 0.12091 \cdot 10^{-7}\, x^{12} + 0.53787 \cdot 10^{-10}\, x^{15} + \cdots$$

Observe that $\boldsymbol{G_n > 0}$ (proof?)

Bad News

The recursive computation of G_n is

unstable

(The computation of the **sum** $\sum_{n=0}^{\infty} G_n x^n$ is stable: no cancellation)

Minimality

G_n is one of the solutions of $\boldsymbol{u_{n+2}} = \dfrac{10\,(n+1)^2\,\boldsymbol{u_{n+1}} - \boldsymbol{u_n}}{(n+1)\,(n+2)\,(3\,n+4)\,(3\,n+5)}$

$$u_n = \frac{v_n}{n!^2} \quad ➡ \quad \boldsymbol{v_{n+2}} = \left(\frac{10}{9} + o(1)\right)\boldsymbol{v_{n+1}} - \left(\frac{1}{9} + o(1)\right)\boldsymbol{v_n}$$

Perron-Kreuser Theorem

$\dfrac{v_{n+1}}{v_n} \to \begin{cases} \text{either } 1 & \text{dominant solution (generic case)} \\ \text{or } 1/9 & \text{minimal solution (non-generic)} \end{cases}$

Experimentally $G_n \approx \dfrac{1}{9^n\,n!^2}$ (minimal!) (proof?)

$\dfrac{1}{9^n\,n!^2} + \varepsilon \cdot \dfrac{1}{n!^2} \approx \varepsilon \cdot \dfrac{1}{n!^2}$ ➡ numerically unstable recursion

Miller's Method

Idea

"Unroll" the recurrence **backwards** for stability

...starting from arbitrary "initial" values

Algorithm

Choose $N \gg 0$

Set $u_N = 1,\ u_{N+1} = 0$

Compute $u_{N-1}, \ldots, u_1, u_0$

using the recurrence

Return the list of $\tilde{G}_n^{(N)} = \dfrac{G_0}{u_0} u_n$

$u_0 = 5.045\ 10^{22}$	➡	$G_0 = 4.475\ 10^{-2}$
$u_1 = 5.679\ 10^{21}$	➡	$G_1 = 5.039\ 10^{-3}$
$u_2 = 1.584\ 10^{20}$	➡	$G_2 = 1.405\ 10^{-4}$
$u_3 = 1.960\ 10^{18}$	➡	$G_3 = 1.739\ 10^{-5}$
$u_4 = 1.363\ 10^{16}$	➡	$G_4 = 1.209\ 10^{-8}$
$u_5 = 6.064\ 10^{13}$	➡	$G_5 = 5.379\ 10^{-11}$
$u_6 = 1.873\ 10^{11}$	➡	$G_6 = 1.661\ 10^{-13}$
$u_7 = 4.248\ 10^{8}$	➡	$G_7 = 3.768\ 10^{-16}$
$u_8 = 7.369\ 10^{5}$	➡	$G_8 = 6.538\ 10^{-19}$
$u_9 = 1000.$	➡	$G_9 = 8.869\ 10^{-22}$
$\boldsymbol{u_{10} = 1.}$	➡	$G_{10} = 8.869\ 10^{-25}$
$\boldsymbol{u_{11} = 0.}$		$G_{11} = 0$

Convergence of Miller's Method

Algorithm

Choose $N \gg 0$

Set $\boldsymbol{u_N = 1,\ u_{N+1} = 0}$ $\leftarrow$ same starting values for all N

Compute $u_{N-1}, \ldots, u_1, u_0$

using the recurrence

Return the list of $\tilde{G}_n^{(N)} = \dfrac{G_0}{u_0} u_n$

Theorem (classical)

For fixed n, we have $\boldsymbol{\tilde{G}_n^{(N)} \to G_n}$ as $\boldsymbol{N \to \infty}$

Final algorithm

1. Compute error bounds, choose working precision (how?)
2. Compute $F(x)$ by direct recurrence
3. Compute $G(x)$ using Miller's method
4. Divide

Numerically stable in practice (proof?)

I didn't yet

prove

anything

Making the Analysis Rigorous

- Prove that (G_n) is a minimal solution
  [$\Rightarrow$ Miller's method works]
- Prove that $G_n \geqslant 0$
  [$\Rightarrow$ no cancellation]

Main issue:

need **bounds on G_n**

- Bound the tails of the series F and G
- Bound the roundoff errors in $\sum F_n x^n$
- Bound the method error of Miller's algorithm
- Bound additional roundoff errors due to Miller's method [M&vdS 1976]

R.M.M. Mattheij & A. van der Sluis, *Numerische Mathematik*, 1976

Controlling G_n

Main Technical Lemma

$$G_n \sim \gamma_n = \frac{1}{4\sqrt{3}\,\pi\, 9^n\, n!^2} \quad \text{with} \quad \left|\frac{G_n}{\gamma_n} - 1\right| \leqslant 2.4\, n^{-1/4} \quad \text{for all} \quad n \geqslant 1$$

Corollary: $G_n > 0$ (for large n, then for all n)

Idea of the proof

- $G_n = \dfrac{1}{2\pi i} \oint \dfrac{G(z)}{z^{3n+1}}\, \mathrm{d}z$
- saddle-point method
- $\mathrm{Ai}(z) \sim \dfrac{e^{-\frac{2}{3} z^{3/2}}}{2\sqrt{\pi}\, z^{1/4}}$ + error bound

Summary

- New well-conditioned formula for $\mathrm{Ai}(x)$, obtained by an extension of the GMR method
- Rigorous error analysis on this example
- Ready-to-use multiple-precision algorithm for $\mathrm{Ai}(x)$

  implementation & suppl. material at http://hal.inria.fr/hal-00767085

Next question: How much of this is specific to $\mathrm{Ai}(x)$?

- Entire function
- Ability to find auxiliary series
- D-finiteness [constraints on the order of the recurrences?]
- Asymptotic estimate with error bound

S. Chevillard & M. Mezzarobba, ARITH 2013

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