Évaluation de $\mathrm{Ai}(x)$

Cancellation catastrophique & comment y échapper

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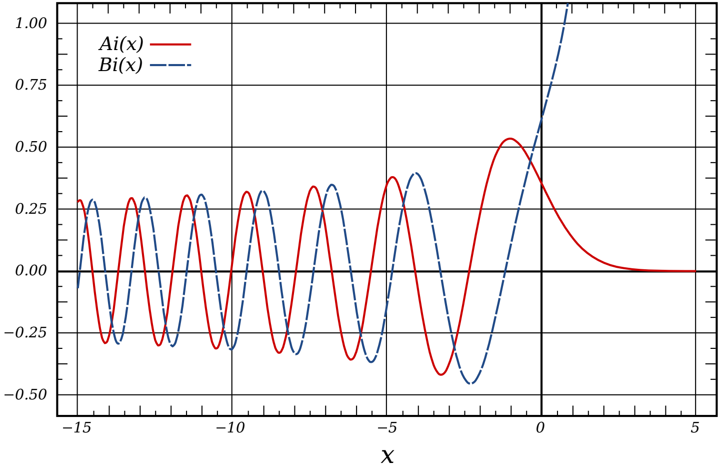
Séminaire SpecFun (Palaiseau), 21 février 2013

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



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

Multiple-Precision Evaluation of $\mathrm{Ai}(x)$, $x > 0$

Standard algorithm

- "Small" x: Taylor Series at 0

  for $n = 0, 1, \ldots, N-1$ (all ops done in floating-point at precision p_{work})
  $t_n := a_1(n) \cdot t_{n-1} \cdot x + a_2(n) \cdot t_{n-1}\, x^2 + \cdots + a_k(n) \cdot t_{n-k} \cdot x^k$
  $s := s + t_n$

  catastrophic cancellation for moderately large x — need $p_{\mathrm{work}} \gg p_{\mathrm{res}}$

- "Large" x (depending on prec.): Asymptotic Expansion at ∞

This talk

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

Complete error analysis (à la MPFR)

Cancellation

Catastrophic Cancellation: A Simple Example

$$\exp(-x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} x^n, \qquad x = 20$$

```
> x := 20: N := 100:
> add((-20.)^n/n!, n=0..99);
```

$$-.12115250e-1$$

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

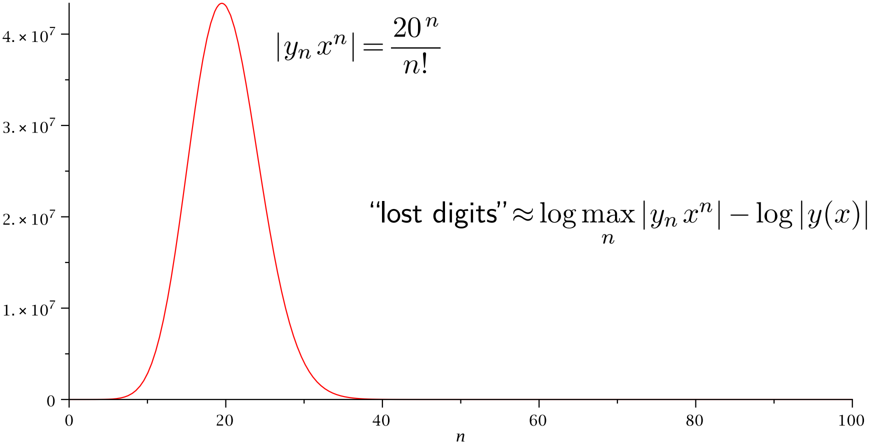
$$.2061153622e-8$$

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

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

$$.206115362243865948417e-8$$

A Simple Example (cont.)



$$|y_n\, x^n| = \frac{20^{\,n}}{n!}$$

$$\text{“lost digits”} \approx \log \max_n |y_n\, x^n| - \log |y(x)|$$

The right way: $\qquad e^{-x} = \dfrac{1}{e^x}$

The Error Function

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

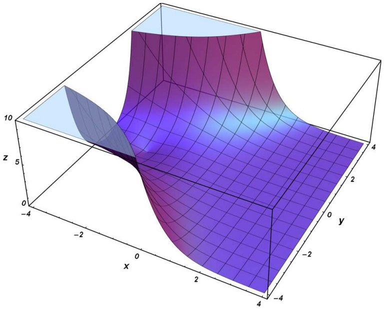
cancellation

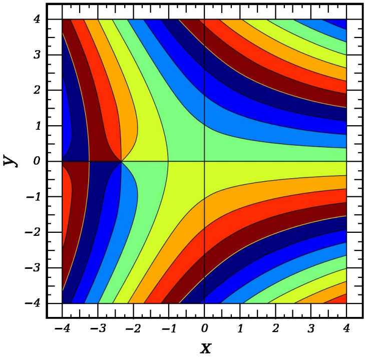
But... (Abramowitz & Stegun, Eq. 7.1.6)

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \exp\left(-x^2\right) \underbrace{\sum_{n=0}^{\infty} \frac{2^n}{1 \cdot 3 \cdots (2\,n+1)}\, x^{2n+1}}_{G(x)}$$

1. Compute $G(x)$ [positive terms, minimal cancellation]
2. Compute $\exp\left(x^2\right)$
3. Divide

Back to Ai(x)





$$\begin{aligned}\mathrm{Ai}(x) &= A - B\,x + \frac{A}{6}\,x^3 - \frac{B}{12}\,x^4 + \frac{A}{180}\,x^6 - \frac{B}{504}\,x^7 + \frac{A}{12960}x^9 + \cdots \\ &= A\sum_{n=0}^{\infty}\frac{1\cdot 4\cdots(3\,n-2)}{(3\,n)!}\,x^{3n} - B\sum_{n=0}^{\infty}\frac{2\cdot 5\cdots(3\,n-1)}{(3\,n+1)!}\,x^{3n+1}\end{aligned}$$

The GMR Method

The Gawronski-Müller-Reinhard Cancellation Reduction Method

- Find F and G such that
  - $y(x) = \frac{G(x)}{F(x)}$
  - The evaluation of F and G involves little cancellation
- Based on the asymptotic behaviour of y at complex ∞
- $\mathrm{Ai}(z) \sim \frac{e^{-\frac{2}{3}z^{3/2}}}{2\sqrt{\pi}\, z^{1/4}}$ as $z \to \infty$

  in any sector $\{z \in \mathbb{C} | -\varphi < \arg z < \varphi\}$ with $\varphi > 0$

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

M. Reinhard. Phd thesis, Universität Trier, 2008.

The Indicator of an Entire Function

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

Order

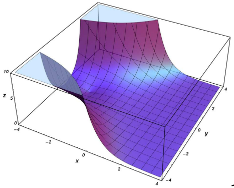
$$\rho = \limsup_{r\to+\infty} \frac{\ln\ln M(r)}{\ln r}$$

Indicator

$$h(\theta) = \limsup_{r\to+\infty} \frac{\ln|y(r\,e^{i\theta})|}{r^\rho}$$

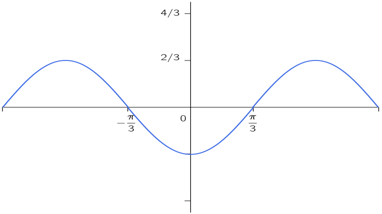
$$|y(r\,e^{i\theta})| \approx \exp\left(\boldsymbol{h}(\theta)\,r^{\boldsymbol{\rho}}\right)$$

for large r



$$\mathrm{Ai}(z) \approx \exp\left(-\frac{2}{3}\,z^{3/2}\right)$$

$$\rho = \frac{3}{2}, \qquad h_{\mathrm{Ai}}(\theta) = -\frac{2}{3}\cos\left(\frac{3}{2}\,\theta\right)$$



Lost in Cancellation

$|y(r\,e^{i\theta})| \approx e^{h(\theta)r^\rho}$ for large r

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

$$
\begin{aligned}
\text{``lost'' digits} \;&\approx\; \log_{10}\Bigl(\max_n |y_n\, z^n|\Bigr) - \log_{10}|y(z)| \\
&\approx\; \log_{10}\frac{M(|z|)}{|y(z)|} \\
&\approx\; \ln\frac{M(|z|)}{|y(z)|} \\
&\approx\; (r^\rho \max_\varphi h(\rho)) - r^\rho\, h(\theta) \qquad (z = r\,e^{i\theta}) \\
&=\; r^\rho\,(\max h - h(\theta))
\end{aligned}
$$

The GMR Method

- "lost" digits $\approx r^\rho\,(\max h - h(\theta))$

- same ρ $\quad\Rightarrow\quad$ $h_{F/G} = h_G - h_F$

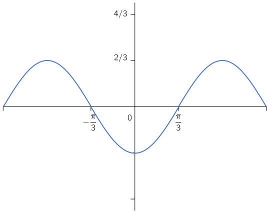
$$\begin{cases} F(z) \approx e^{h_F(\theta) r^\rho} \\ G(z) \approx e^{h_G(\theta) r^\rho} \end{cases} \quad\Rightarrow\quad \frac{G(z)}{F(z)} \approx \exp\left[(h_G(\theta) - h_F(\theta))\, r^\rho\right]$$

- **Idea:** look for
  - an auxiliary series F
  - a modified series $G = y\,F$

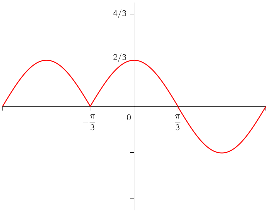
  such that h_F and h_G $\approx$ their max for $\theta = 0$

Auxiliary Series for $\mathrm{Ai}(x)$

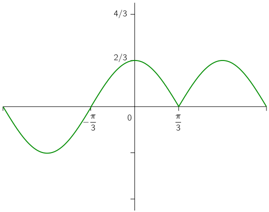
Indicators



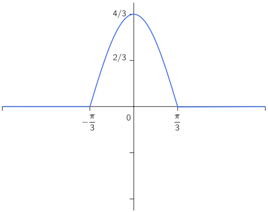
$\mathrm{Ai}(x)$



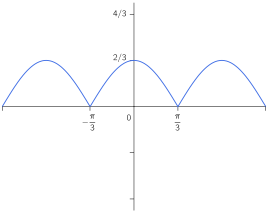
$\mathrm{Ai}(j^{-1}\,x)$



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



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



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

The Auxiliary Series $F(x)$

$$F(x) = \mathrm{Ai}(j\,x)\,\mathrm{Ai}(j^{-1}\,x) = \frac{1}{4}\left(\mathrm{Ai}(x)^2 + \mathrm{Bi}(x)^2\right) = \sum F_n\,x^n$$

D-Finiteness

$$\mathrm{Ai}''(x) - x\,\mathrm{Ai}(x) = 0 \quad \rightsquigarrow \quad \boldsymbol{F_{n+3}} = \frac{2\,(2\,n+1)}{(n+1)\,(n+2)\,(n+3)}\,\boldsymbol{F_n}$$

$$\mathrm{Ai}(0) = A \quad \mathrm{Ai}'(0) = B$$

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

$$F_2 = \frac{1}{3^{2/3}\,\Gamma\left(\frac{1}{3}\right)^2}$$

- Two-term recurrence $\Rightarrow$ Easy to evaluate
- Obviously $F_n > 0$ $\Rightarrow$ No cancellation

The Modified Series $G(x)$

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

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

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

$$G(x) = 0.44749 \cdot 10^{-1} + 0.50371 \cdot 10^{-2}\, x^3 + .14053 \cdot 10^{-3}\, x^6 + .17388\, 10^{-5}\, x^9 + .12091 \cdot 10^{-7}\, x^{12} + .53787 \cdot 10^{-10}\, x^{15} + \cdots$$

Note: Prove that $G_n > 0$?

Are We Done Yet?

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

Perron-Kreuser

$u_n = \dfrac{v_n}{n!^2}$

where

$$\frac{u_{n+1}}{u_n} \to \begin{cases} \quad 1 & \text{dominant solution — generic case} \\ \text{or} \quad 1/9 & \text{minimal solution — non-generic} \end{cases}$$

Experimentally $G_n \approx \dfrac{1}{9^n\, n!^2}$ Minimal sol. $\Longrightarrow$ unstable recursion

Miller's Method

Idea

"Unroll" the recurrence backwards; then minimal $\rightsquigarrow$ dominant

Algorithm

Choose $N \gg 0$
Set $u_N = 1$, $u_{N+1} = 0$
Compute $u_{N-1}, \ldots, u_1, u_0$
Return the list of $\tilde{c}_n^{(N)} = \frac{c_0}{u_0} u_n$, $n = 0, 1, \ldots$

Theorem (classical)

For fixed n, we have $\tilde{c}_n \to c_n$ as $N \to \infty$

\+ Numerically stable

Evaluation Algorithm

1. Compute $F(x)$ by direct recurrence
2. Compute $G(x)$ using Miller's method
3. Divide

Works well in practice.

Proof?

Error bounds?

Proofs & Error Bounds

What Remains To Do

- Prove that (G_n) is a minimal solution

  (i.e. the one to which Miller's method converges)
- Prove that $G_n \geqslant 0$ (so that the summation is numerically stable)

- Bound the tails of the series F and G [easy]
- Bound the roundoff errors in $\sum F_n x^n$ [tedious but routine]
- Bound the method error of Miller's algorithm (i.e. $|G_n - n!^{-2}\,\tilde{c}_n^{(N)}|$)

  ⇝ Main issue: **need bounds on G_n**
- Bound the corresponding additional roundoff errors

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

Controlling G_n

Proposition

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

Idea of the proof

- $G_n = \dfrac{1}{2\,\pi\,i} \oint \dfrac{G(z)}{z^{3n+1}}\,\mathrm{d}z$
- saddle-point method
- $\mathrm{Ai}(z) \sim \dfrac{e^{-\frac{2}{3}z^{3/2}}}{2\sqrt{\pi}\,z^{1/4}} =: \widetilde{\mathrm{Ai}}(z),$ $\left|\dfrac{\mathrm{Ai}(z)}{\widetilde{\mathrm{Ai}}(z)} - 1\right| \leqslant r^{-3/2}\,\dfrac{5}{48}\cos\dfrac{\theta}{2}$

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

Conclusion

Summary

- New well-conditioned formula for $\mathrm{Ai}(x)$,

  obtained by an extension of the GMR method
- Detailed example of how to make the method rigorous
- Ready-to-use multiple-precision algorithm for $\mathrm{Ai}(x)$

How much of this all 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

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