

Fast and accurate algorithm for the generalized exponential integral $E_\nu(x)$ for positive real order



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Abstract

We describe an algorithm for the numerical evaluation of the generalized exponential integral $E_\nu(x)$ for positive values of ν and x . The performance and accuracy of the resulting algorithm is analysed and compared with open-source software packages. This analysis shows that our implementation is competitive and more robust than other state-of-the-art codes. The described algorithm is part of the author's library Chypergeo.

Introduction

The generalized exponential integral is defined by

$$E_\nu(x) = \int_1^\infty e^{-xt} t^{-\nu} dt, \quad \nu \in \mathbb{R}, x > 0.$$

The function $E_\nu(x)$, with $\nu > 0$, appears in many fields of physics and engineering, in particular is of interest its connection with transport theory and radiative equilibrium. The generalized exponential integral plays an important role in some exponentially-improved asymptotic expansions for the confluent hypergeometric function $U(a, b, x)$ [1].

Methods of computation

The algorithm combines the use of series expansions, Laguerre series and asymptotic expansions. A detailed description of methods used in each region is presented in [2].

► Power series:

► option 1 [1, §8.19.10]

$$E_\nu(x) = \Gamma(1-\nu)x^{\nu-1} - \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{(1-\nu+k)k!}, \quad \nu \in \mathbb{R} \setminus \mathbb{N}, x \neq 0$$

► option 2 (more numerically stable for small ν) [1, §8.19.11]

$$E_\nu(x) = \Gamma(1-\nu)x^{\nu-1} + \frac{e^{-x}}{\nu-1} \sum_{k=0}^{\infty} \frac{x^k}{(2-\nu)_k}$$

► Laguerre series [2, §2.2.2]

► Globally convergent series. Does not exhibit significant cancellation.
► Small number of terms required for moderate x .

$$E_\nu(x) = e^{-x} \sum_{k=0}^{\infty} \frac{(\nu)_k}{(k+1)! L_k^{(\nu-1)}(-x) L_{k+1}^{(\nu-1)}(-x)}$$

► The generalized Laguerre polynomials satisfy the three-term recurrence relation

$$L_{k+1}^{(\nu-1)}(-x) = \frac{x+2k+\nu}{k+1} L_k^{(\nu-1)}(-x) - \frac{k+\nu-1}{k+1} L_{k-1}^{(\nu-1)}(-x).$$

► Special cases

► $n \in \mathbb{N}$ [1, §8.19.8] and [1, §8.19.7]

$$E_n(x) = \frac{(-x)^{n-1}}{(n-1)!} (\psi_0(n) - \log(x)) - \sum_{k=0, k \neq n-1}^{\infty} \frac{(-x)^k}{k!(1-n+k)}$$

$$E_n(x) = \frac{(-x)^{n-1}}{(n-1)!} E_1(x) + e^{-x} \sum_{k=0}^{n-2} (n)_{-k-1} (-x)^k$$

► Special case for $n+1/2$, $n \in \mathbb{N}$ is also included.

► Other numerical methods such as continued fractions or numerical integration have been studied, but they were ultimately discarded.

Asymptotic expansions

► Large x and fixed ν [1, §8.20(i)]

► It is derived from the integral representation using Watson lemma.

$$E_\nu(x) \sim e^{-x} \sum_{k=0}^{\infty} \frac{(-1)^k (\nu)_k}{x^{k+1}}$$

► Large ν and fixed x [2, §2.3.3]

► It is derived from the integral representation

$$E_\nu(x) = e^{-x} \int_0^\infty e^{-\nu t} f(t) dt, \quad f(t) = e^{t-x(e^t-1)}$$

after performing a change of variable and interchanging summation and integration we have

$$E_\nu(x) \sim -\frac{e^{-x}}{x} \sum_{k=0}^{\infty} \frac{B_{k+1}(-x)}{\nu^{k+1}}, \quad \nu \rightarrow \infty.$$

► Bell polynomials $B_n(x)$ can be defined by Cauchy's integral formula

$$B_n(x) = \frac{n!}{2\pi i} \int_C \frac{e^{x(z^2-1)}}{z^{n+1}} dz = \frac{n!}{2\pi} \int_0^{2\pi} e^{x(e^{it}-1)} e^{-int} dt.$$

and satisfy the following saddle point bound

$$|B_n(x)| \leq \lambda \left| \frac{n! e^{xW(n/x)}}{2\pi e^x W(n/x)^n} \right|,$$

where

$$\lambda = |0 - t_0| + |2\pi - t_0| \quad \text{and} \quad t_0 = -i(\log(n/x) - W(n/x)),$$

and $W(x)$ is the Lambert- W function.

Uniform asymptotic expansion

► Large ν and x [1, §8.20(ii)]

$$E_\nu(x) \sim \frac{e^{-z}}{x+\nu} \sum_{k=0}^{\infty} \frac{A_k(\lambda)}{(\lambda+1)^{2k} \nu^k}.$$

where $\lambda = x/\nu$. $A_k(\lambda)$ is an Eulerian polynomial of second kind defined by

$$A_k(\lambda) = \sum_{m=0}^k (-1)^m \left\langle \left\langle \begin{matrix} k \\ m \end{matrix} \right\rangle \right\rangle \lambda^m,$$

where $\left\langle \left\langle \begin{matrix} k \\ m \end{matrix} \right\rangle \right\rangle$ are second-order Eulerian numbers, defined by the recursion equation

$$\left\langle \left\langle \begin{matrix} k \\ m \end{matrix} \right\rangle \right\rangle = (m+1) \left\langle \left\langle \begin{matrix} k-1 \\ m \end{matrix} \right\rangle \right\rangle + (2k-m-1) \left\langle \left\langle \begin{matrix} k-1 \\ m-1 \end{matrix} \right\rangle \right\rangle.$$

Results: Benchmark - statistics

► Case: $\nu \in \mathbb{N}$

| Library | Max. error | Avg. error | Avg. time (μs) | Stdev. time (μs) | fails |
|--------------|------------|------------|-----------------------|-------------------------|--------|
| Chypergeo | 9.7e-16 | 1.3e-16 | 0.25 | 0.21 | 0/200 |
| Cephes | 1.4e-15 | 2.0e-16 | 0.73 | 2.47 | 0/200 |
| Boost-1.61.0 | 4.8e-15 | 3.3e-16 | 63.76 | 558.36 | 0/200 |
| GSL-2.2.1 | 5.2e-14 | 6.1e-15 | 1.34 | 1.19 | 75/200 |

► Case: $\nu \in \mathbb{R}^+$. Two sample sets with the following characteristics:

- Large set: $\nu \in [0, 10000]$ and $x \in [1.0e-9, 1000]$
- Small set: $\nu \in [0.04, 70]$ and $x \in [0.00075, 1.5]$

| Library | Max. error | Avg. error | Avg. time (μs) | Stdev. time (μs) | fails |
|-----------|------------|------------|-----------------------|-------------------------|--------|
| Large set | 9.8e-16 | 1.1e-16 | 0.14 | 0.10 | 0/1500 |
| Small set | 3.1e-15 | 1.7e-16 | 0.52 | 0.37 | 0/500 |

► Error statistics for each library. gcc-5.4.0 compiler running Cygwin. Time in microseconds. Fails: returns Incorrect/NaN/Inf. Intel(R) Core(TM) i5-3317 CPU at 1.70GHz.

Results: Benchmark - profiles

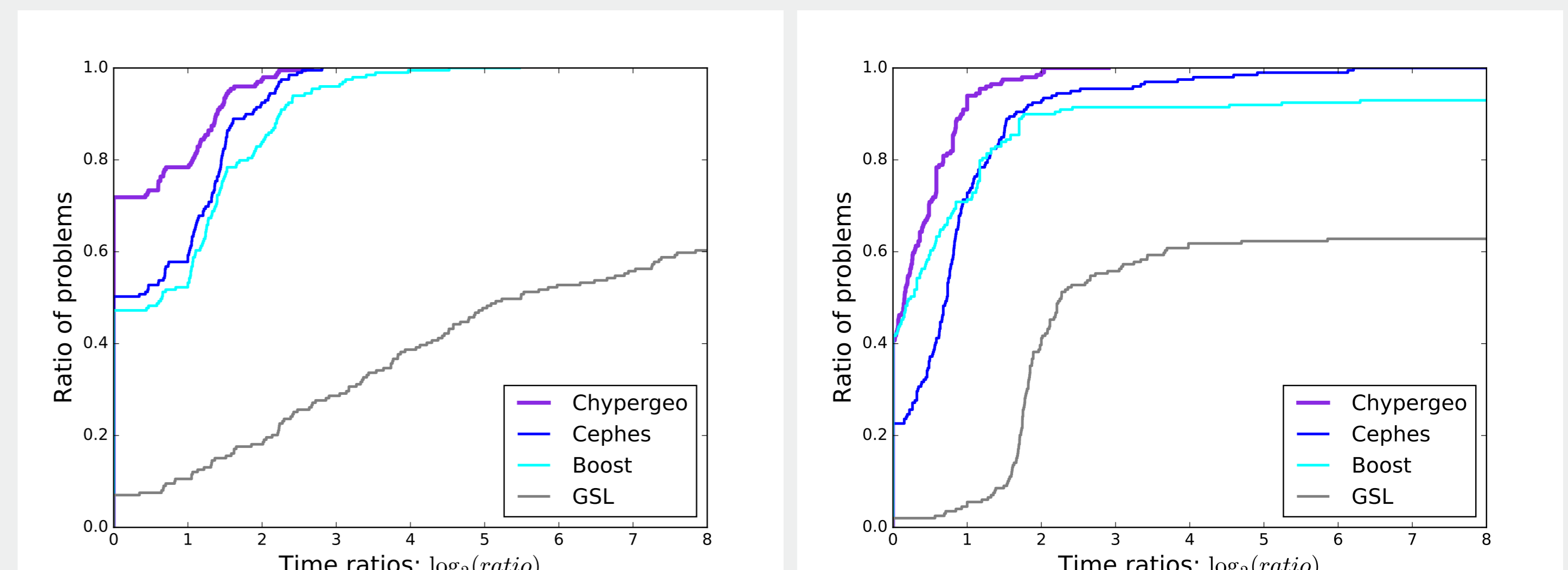


Figure 1: Case $\nu \in \mathbb{N}$. Accuracy profiles (left). Performance profiles (CPU time) (right). The algorithm outperforms the other codes. GSL shows very poor results.

Conclusion

- New implementation outperforms available software packages in terms of accuracy and computation time.
- Includes a new asymptotic expansion for large order ν and other methods not implemented in existing software.
- Use of internal higher precision arithmetic (Error free transformation + double-double arithmetic) for regions showing numerical instability.

References

- [1] NIST Digital Library of Mathematical Functions. <http://dlmf.nist.gov/>, Release 1.0.14 of 2016-12-21.
- [2] G. Navas-Palencia. *Fast and accurate algorithm for the generalized exponential integral $E_\nu(x)$ for positive real order*. Numerical Algorithms (2017).

Chypergeo Library

► Features

- C++ library for fast and accurate evaluation of special functions in double precision arithmetic. It supports real and complex values.
- Fast and efficient multi-evaluation of special functions with OpenMP.
- Web: sites.google.com/site/guillermonavaspalencia/software/chypergeo
- GNSTLIB is a numerical library extending Chypergeo. GNSTLIB is a joint work with Amparo Gil, Javier Segura and Nico M. Temme.