High-precision computation of uniform asymptotic expansions for special functions

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Confluent hypergeometric functions and derived cases

- Main definition

$$z\frac{d^2w}{dz^2} + (b-z)\frac{dw}{dz} - aw = 0. \quad \text{(Kummer's equation)}$$

Name	Notation
Confluent hypergeometric function	${}_1F_1(a;b;z)$, $U(a,b,z)$ and ${}_0F_1(-;b;z)$
Exponential, logarithmic and trigonometric integrals	$\mathrm{Ei}(z)$, $\mathrm{E}_1(z)$, $\mathrm{li}(z)$, $\mathrm{Si}(z)$, $\mathrm{Ci}(z), \ldots$
Error functions, Dawson's and Fresnel integrals	$\mathrm{erf}(z)$, $\mathrm{erfc}(z)$, $\mathrm{erfi}(z)$, $S(z)$, $C(z), \ldots$
Incomplete Gamma and generalized exponential integral	$\Gamma(a,z)$, $\gamma(a,z)$, $E_\nu(z)$ and ratios
Airy functions	$\mathrm{Ai}(z)$, $\mathrm{Ai}'(z)$, $\mathrm{Bi}(z)$ and $\mathrm{Bi}'(z)$
Bessel functions	$J_\nu(z)$, $Y_\nu(z)$, $I_\nu(z)$ and $K_\nu(z)$
Parabolic cylinder functions	$U(a,z)$, $U'(a,z)$, $V(a,z)$ and $V'(a,z)$
Orthogonal polynomials	$L_\nu^\alpha(z)$ and $H_\nu(z)$

The Lerch transcendent

Lerch transcendent and derived cases

- Primary definition

$$\Phi(z,s,a) = \sum_{k=0}^{\infty} \frac{z^k}{(k+a)^s},$$

where $a \notin \mathbb{Z}_0^-$, $|z| < 1$ or $\Re(s) > 1$, $|z| = 1$.

Name	Notation
Lerch transcendent	$\Phi(z,s,a)$
Riemann zeta function	$\zeta(s) = \Phi(1,s,1)$
Hurwitz zeta function	$\zeta(s,a) = \Phi(1,s,a)$
Polylogarithm	$\text{Li}_s(z) = z\Phi(z,n,1)$
Periodic zeta function	$E_s(z) = \Phi(e^{2\pi iz},s,1)$
Generalized L-series	Dirichlet series and others

Table: Lerch transcendent and main derived cases.

Software Development for Special Functions

Arithmetic and software

Arithmetic

- Arbitrary-precision arithmetic.
- Floating-point arithmetic.
- Floating-point expansions and error-free transformations.

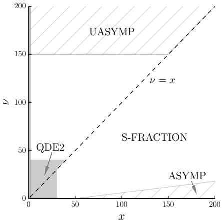
Numerical libraries

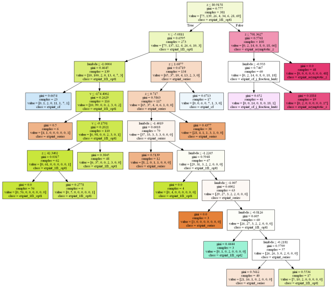
- Arbitrary-precision arithmetic
  - Computer Algebra Systems (CAS): Magma, Maple, Mathematica, SageMath.
  - Libraries: GMP (C/C++), MPFR (C), MPC (C), mpmath (python), Arb (C).
- Double-precision arithmetic
  - Open-source: AMOS, SLATEC, SPECFUN (Fortran), Cephes, GSL (C), Boost (C++), GNSTLIB (C/C++/Python/Fortran).
  - Commercial: IMSL, NAG.

Design of software for computing special functions

Methodology

- Double-precision, all function's domain correctly covered.
- Combine various methods.
- Use of connection formulas and special cases.
- Extended precision to mitigate catastrophic cancellation.
- Rigorous error bounds (heuristic error estimates).
- Determination of the region of applicability for each method.
- How to choose the most suitable method for a region?
  - Numerical analysis of error bounds.
  - Decision trees.
- Vectorized versions.





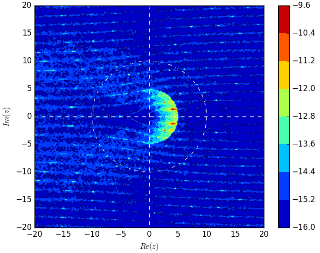
Testing and benchmarking methodologies

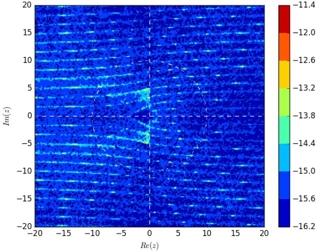
Testing

- Absolute/relative accuracy.
- Efficiency and computation time.
- Plotting $\Longrightarrow$ regions with low accuracy.
- Robustness and stable performance $\Longrightarrow$ portability.
- Use automatic testing tools (Jenkins/Travis).

Benchmarking

- Absolute/relative error statistics.
- Performance profiles.
- Shifted geometric mean.





Generalized Exponential Integral

Journal articles

1. G. Navas-Palencia. *Fast and accurate algorithm for the generalized exponential integral $E_\nu(x)$ for positive real order*. Numerical Algorithms, 77(2):603-630, 2018.

Introduction

The generalized exponential integral is defined by

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

- Applications of $E_\nu(x)$, with $\nu > 0$
  - Physics: transport theory and radiative equilibrium.
  - Mathematics: exponentially-improved asymptotic expansions.
- Relevant works
  - Chiccoli, Lorenzutta and Maino (1987, 1990, 1992).

Objective

- Fast and reliable algorithm for $\nu \in \mathbb{R}^+$ and $x > 0$. Partial use of double-double arithmetic.
- Improve accuracy in difficult regions of computation.
- New asymptotic expansion for $\nu \to \infty$.

Methods of computation

- Power series. Two options: alternating series and series with positive terms for $\nu < 2$.
- Laguerre series
  - Globally convergent series. Does not exhibits 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

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

- Taylor series for $1 \leq x < 2$.
- Several special cases for $\nu = n$ and $\nu = n + 1/2$, $n \in \mathbb{N}$.
- Special case: $n + \epsilon$, $n \in \mathbb{N}$:
  - Difficult case arises when $\nu = n + \epsilon$, $|\epsilon| \ll 1$, for small values of x.
  - Significant loss of precision both in the series expansion and $\Gamma(1 - n - \epsilon)x^{n-1+\epsilon}$.
  - Series expansions implemented in quadruple precision (128-bit) using the libquadmath.
  - Interface `expint(const double v, const double x)`, where `vi` and `vf` ($|$`vf`$| < 0.5$).
  - Quadruple precision is about $10 \sim 15$ times slower.

Methods of computation (uniform asymptotic expansion)

- Uniform asymptotic expansion for large ν and x in terms of Eulerian polynomial of second kind $A_k(\lambda)$

$$E_\nu(x) \sim \frac{e^{-z}}{x+\nu} \sum_{k=0}^{\infty} \frac{A_k(\lambda)}{(\lambda+1)^{2k}\nu^k}, \quad A_k(\lambda) = \sum_{m=0}^{k} (-1)^m \left\langle\!\!\left\langle {k \atop m} \right\rangle\!\!\right\rangle \lambda^m,$$

where $\lambda = x/\nu$. Coefficients $\left\langle\!\left\langle {k \atop m} \right\rangle\!\right\rangle$ are second-order Eulerian numbers, defined by the recursion equation

$$\left\langle\!\!\left\langle {k \atop m} \right\rangle\!\!\right\rangle = (m+1) \left\langle\!\!\left\langle {k-1 \atop m} \right\rangle\!\!\right\rangle + (2k-m-1) \left\langle\!\!\left\langle {k-1 \atop m-1} \right\rangle\!\!\right\rangle.$$

  - Introduced by Gautschi (1959), computing coefficients $A_k(\lambda)$ via recursion involving derivatives

$$A_{k+1}(\lambda) = (1-2k\lambda)A_k(\lambda) + \lambda(\lambda+1)\frac{dA_k(\lambda)}{d\lambda}, \quad k = 0, 1, 2, \ldots$$

  - Efficient computation of Eulerian polynomials of the second kind $\Longrightarrow$ suitable for arbitrary-precision arithmetic.
  - For fixed precision pre-compute polynomials. Evaluation using Horner's scheme and compensated summation algorithms.

Methods of computation (new asymptotic expansion)

Proposition

Asymptotic expansion for large ν and fixed x in terms of Bell polynomials $B_n(x)$,

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

Theorem (Uniform bound for Bell polynomials $B_n(x)$)

The Bell polynomials can be defined by Cauchy's integral formula

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

and satisfy

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

where

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

Benchmark

Benchmark settings

- gcc-5.4.0 compiler running Cygwin.
- Intel(R) Core(TM) i5-3317 CPU at 1.70GHz.

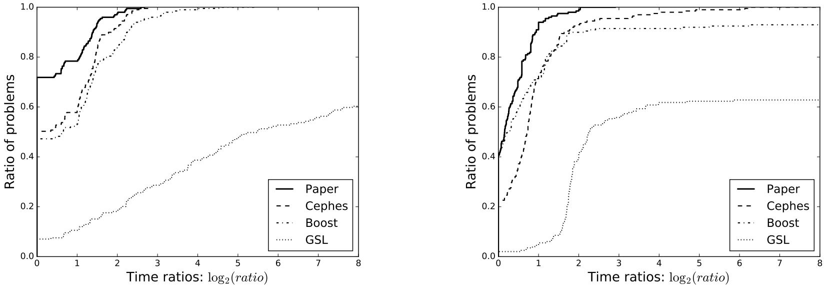


Figure: Accuracy and performance profiles case $n \in \mathbb{N}$ and $x > 0$.

Library	Max. error	Avg. error	Avg. time (μs)	Stdev. time (μs)	fails
Paper	**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

Table: Error statistics for each library. Time in microseconds. Fails: returns Incorrect/NaN/Inf.

Confluent Hypergeometric Functions

Journal articles

1. G. Navas-Palencia and A. Arratia. *On the computation of confluent hypergeometric functions for large imaginary part of parameters b and z*. Lecture Notes in Computer Science, 9725:241–248, 2016.
2. G. Navas-Palencia. *High-precision computation of the confluent hypergeometric functions via Franklin-Friedman expansion*. Advances in Computational Mathematics, 44(3):841-859, 2018.

Introduction

The confluent hypergeometric function of the first kind $M(a,b,z) = {}_1F_1(a;b;z)$ arises as one of the solutions of the limiting form of the hypergeometric differential equation

$$z\frac{d^2w}{dz^2} + (b-z)\frac{dw}{dz} - aw = 0, \quad b \notin \mathbb{Z}_0^-.$$

Another standard solution is the confluent hypergeometric function of the second kind $U(a,b,z)$, $U(a,b,z) \sim z^{-a},\ z \to \infty,\ |\mathrm{ph}\, z| \le (3/2)\pi$.

- Power series

$$ {}_1F_1(a;b;z) = \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k k!} z^k.$$

- Integral representation

$$U(a,b,z) = \frac{1}{\Gamma(a)} \int_0^{\infty} t^{a-1} e^{-zt} (1+t)^{b-a-1}\, dt, \quad \Re(a) > 0,\ \Re(z) > 0.$$

- Numerical libraries double-precision arithmetic combine various numerical methods.
  - Series expansions.
  - Asymptotic expansions for large argument or parameters (or both).
  - Numerical quadrature.
- Applications: Physics, mathematics and statistics, among others.

Computation for large imaginary part of parameters b and z

- High oscillatory integrals commonly encountered in the form of Fourier-type integrals.
- Methods: stationary phase, Filon-type, Levin, complex-valued Gaussian quadrature and specialized double-exponential quadratures, etc..
- Numerical steepest descent method. Huybrechs and Vandewalle (2006).

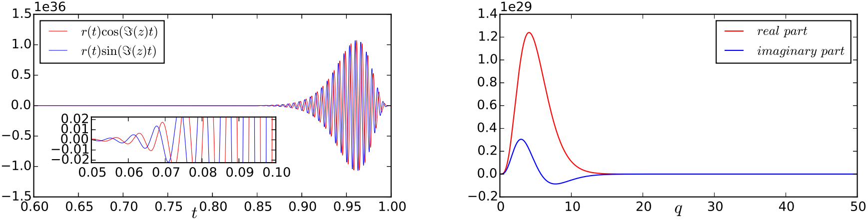


Figure: Real and imaginary part of integrand for ${}_1F_1(5, 10, 100 - 1000i)$ before and after applying steepest descent method.

- Applications
  - Statistics: characteristic functions of several probability distributions; e.g., beta and F-distribution.
  - Finance: computation of Asian options and credit risk models.

Integrals for large imaginary part of parameters b and z for $U(a,b,z)$

- Case $U(a,b,z)$, $\Im(z) \to \infty$

$$U(a,b,z) = \frac{i}{\omega\Gamma(a)} \int_0^{\infty} e^{-\Re(z) i \frac{q}{\omega}} \left(i\frac{q}{\omega}\right)^{a-1} \left(1 + i\frac{q}{\omega}\right)^{b-a-1} e^{-q}\, dq,$$

where $\omega = -\Im(z)$.

- Case $U(a,b,z)$, $\Im(b) \to \infty$

$$U(a,b,z) = \frac{ie^{z}}{\omega\Gamma(a)} \int_0^{\infty} e^{\phi(q,\omega)} (e^{\mu(q,\omega)} - 1)^{a-1} \left(e^{\mu(q,\omega)}\right)^{\Re(b)-a-1} e^{-q}\, dq,$$

where $\omega = \Im(b)$, $\mu(q,\omega) = i\frac{q}{\omega}$ and $\phi(q,\omega) = -ze^{\mu(q,\omega)} + \mu(q,\omega)$.

Integrals for large imaginary part of parameters b and z for ${}_1F_1(a;b;z)$

- Case ${}_1F_1(a,b,z)$, $\Im(z) \to \infty$

$$
\begin{aligned}
{}_1F_1(a;b;z) &= \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \frac{i}{\omega} \left[\int_0^\infty e^{\Re(z) i \frac{q}{\omega}} \left(i \frac{q}{\omega} \right)^{a-1} \left(1 - i \frac{q}{\omega} \right)^{b-a-1} e^{-q} \, dq \right. \\
& \left. - e^{i\omega} \int_0^\infty e^{\Re(z)(1 + i \frac{q}{\omega})} \left(1 + i \frac{q}{\omega} \right)^{a-1} \left(- i \frac{q}{\omega} \right)^{b-a-1} e^{-q} \, dq \right],
\end{aligned}
$$

where $\omega = \Im(z)$.

- Case ${}_1F_1(a,b,z)$, $\Im(b) \to \infty$
  - Use connection formula valid for all $z \neq 0$.
  - Integral representation rewritten as a Laplace-type integral for large b as follows

$$
{}_1F_1(a;b;z) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^\infty e^{\Re(b)t} (1 - e^{-t})^{a-1} e^{at + z(1-e^{-t})} e^{-i\Im(b)t} \, dt \, .
$$

Benchmarks

Benchmark settings

- Intel(R) Core(TM) i5-3317U CPU at 1.7GHz.
- Algorithm 707: CONHYP (Fortran 90). Nardin, Perger and Bhalla (1992).
- Zhang and Jin algorithm (Fortran 90). Zhang and Jin (1996).
- NSD (Python 3.5.1).

${}_1F_1(a,b,z)$	CONHYP	ZJ	NSD	N
$(1,4,50i)$	3.96e−13/4.29e−18i	1.50e−15/4.28e−18i	1.15e−16/1.11e−16i	2
$(3,10,30+100i)$	1.27e−13/1.28e−13i	6.83e−17/1.07e−14i	2.48e−17/1.24e−14i	25
$(15,20,200i)$	9.20e−13/9.20e−13i	E	8.43e−16/7.93e−16i	25
$(400,450,1000i)$	8.32e−12/1.00e−11i	−	1.37e−12/1.02e−13i	50
$(2,20,50-2500i)$	1.35e−11/1.35e−11i	7.30e−11/2.10e−09i	4.75e−16/6.41e−16i	20
$(500,510,100-1000i)$	4.10e−13/3.68e−12i	−	4.71e−13/3.11e−16i	50
$(2,20,-20000i)$	−	5.79e−10/7.99e−07i	5.92e−16/3.62e−14i	10
$(900,930,-10^{10}i)$	−	−	6.78e−13/6.77e−13i	20
$(4000,4200,50000i)^*$	−	−	6.04e−12/5.99e−12i	80

Table: Relative errors for routines computing the confluent hypergeometric function for complex argument. N: number of Gauss-Laguerre quadratures. $(*)$: precision in `mpmath` increased to 30 digits. (E): convergence to incorrect value. $(-)$: overflow.

Function	Min	Max	Mean
$U(a,b,iz)$	1.97e−18/2.04e−17i	9.97e−13/2.50e−11i	1.34e−14/6.94e−14i
$U(a,ib,z)$	6.57e−18/6.17e−18i	1.49e−11/8.55e−12i	1.38e−13/1.43e−13i

Table: Error statistics for $U(a,b,iz)$ and $U(a,ib,z)$ using $N=100$ quadratures.

The Franklin-Friedman expansion

J. Franklin and B. Friedman developed in 1957 a method for obtaining convergent asymptotic representations for Laplace-type integrals of the form

$$F_\lambda(z) = \frac{1}{\Gamma(\lambda)} \int_0^\infty t^{\lambda-1} e^{-zt} f(t)\, dt, \quad \Re(z) > 0,\ \Re(\lambda) > 0,$$

for large values of z with suitable assumptions on the amplitude function $f(t)$.

Theorem (J. Franklin and B. Friedman, 1957)

$$F_\lambda(z) = \sum_{k=0}^{n-1} f_k(t_k) \frac{(\lambda)_k}{z^{\lambda+2k}} + \frac{1}{z^n \Gamma(\lambda)} \int_0^\infty t^{\lambda+n-1} e^{-zt} f_n(t)\, dt,$$

where $n = 0, 1, 2, \ldots$, $f_0(t) = f(t)$ *and*

$$f_{k+1}(t) = \frac{d}{dt} \frac{f_k(t) - f_k(t_k)}{t - t_k}, \quad t_k = \frac{\lambda + k}{z}, \quad k = 0, 1, 2, \ldots.$$

R. B. Paris, *Hadamard expansions and hyperasymptotic evaluation*, (2011)

"Although the expansion is more accurate than that obtained from Watson's lemma, it suffers from the disadvantage that the coefficients are much more complicated."

The Franklin-Friedman expansion for $U(a,b,z)$

- Asymptotic expansion valid for $|z| \to \infty$, Watson's lemma to the Laplace-type integral.

$$U(a,b,z) \sim z^{-a} \sum_{k=0}^{\infty} (-1)^k \frac{(a)_k (a-b+1)_k}{k! z^k}, \quad |\mathrm{ph}\, z| < \frac{3}{2}\pi,$$

where $(a)_k = a(a+1)\cdots(a+k-1)$.

- Connection formulas for confluent hypergeometric functions for $(a,b,z) \in \mathbb{C}^3$

$${}_1\tilde{F}_1(a;b;z) = \frac{e^{\mp\pi i a}}{\Gamma(b-a)} U(a,b,z) + \frac{e^{\pm i(b-a)}}{\Gamma(a)} e^z U(b-a,b,ze^{\pm\pi i}),$$

- Other methods to obtain uniform asymptotic expansions
  - Vanishing saddle point. N. M. Temme (1983, 1985).
  - Exponentially-improved and hyperasymptotic expansions. F. W. J. Olver (1991, 1995).
  - Hadamard series. R. B. Paris (2009).

Objective

- Closed-form Franklin-Friedman expansion coefficients for Laplace-type integrals with amplitude function $f(t) = (1+t)^{b-a-1}$.

The Franklin-Friedman expansion for $U(a,b,z)$

Theorem (G. Navas-Palencia, 2018)

For $(a,b,z) \in \mathbb{C}^3$ *and* $\Re(z) > 0$ *the Franklin-Friedman expansion for the confluent hypergeometric function* $U(a,b,z)$ *is given by*

$$U(a,b,z) = \sum_{k=0}^{\infty} c_k(z) \frac{(a)_k}{k! z^{a+k}},$$

where

$$\begin{aligned} c_k(z) &= \sum_{j=0}^{k} \binom{k}{j} z^{k-j} \frac{\Gamma(b-a)}{\Gamma(b-a-j)} \sum_{s=j}^{k} (-1)^{s-j} \binom{k-j}{k-s} A_s^{b-a-1-j} \\ &= \sum_{j=0}^{k} \binom{k}{j} z^{j} \frac{\Gamma(b-a)}{\Gamma(b-a+j-k)} \sum_{s=0}^{j} (-1)^{s} \binom{j}{s} A_{k-j+s}^{b-a-1-k+j}, \quad k = 0,1,2,\ldots, \end{aligned}$$

and

$$A_s^q = \left(1 + \frac{a+s}{z}\right)^q.$$

The Franklin-Friedman expansion for $U(a, b, z)$ (proof sketch)

- Compute first coefficients f_k, factorizing and rearranging coefficients $A_s^q := (1 + (a+s)/z)^q$. Proof by induction.

$$f_k = c_k(z) \frac{z^k}{k!},$$

where

$$c_k(z) = \sum_{j=0}^{k} \binom{k}{j} z^{k-j} \frac{\Gamma(b-a)}{\Gamma(b-a-j)} \sum_{s=j}^{k} (-1)^{s-j} \binom{k-j}{k-s} A_s^{b-a-1-j}, \quad k = 0, 1, 2, \ldots$$

- $c_k(z)$ can be written as

$$c_k(z) = z^{k-q} k! \sum_{j=0}^{k} \binom{q}{k-j} \frac{1}{j!} \sum_{s=0}^{j} (-1)^s \binom{j}{s} \frac{1}{(p+k-j+s)^{k-q-j}},$$

where $q = b - a - 1$ and $p = z + a$.

- Integral representation alternating binomial sum (Coffey, 2007).

The Franklin-Friedman expansion for $U(a,b,z)$ (proof sketch)

- Integral representation of $c_k(z)$

$$c_k(z) = \frac{\Gamma(q+1)\sin(\pi(k-q))}{z^{q-k}\pi} \int_0^\infty t^{-q-1} e^{-(p+k)t} (1 - e^t + t)^k \, dt,$$

valid for $\Re(q) < 0$ and $\Re(p) > 0$.

- Interchanging summation and integration

$$\sum_{k=0}^{\infty} \frac{c_k(z)(a)_k}{k! z^{a+k}} = \frac{\Gamma(q+1)}{\pi z^{a+q}} \int_0^\infty \left(\sum_{k=0}^{\infty} \frac{(a)_k \sin(\pi(k-q))(1-e^t+t)^k}{e^{kt} k!} \right) t^{-q-1} e^{-pt} \, dt \, .$$

- Use identity

$$\sum_{k=0}^{\infty} \frac{(a)_k \sin(\pi(k-q))(1-e^t+t)^k}{e^{kt} k!} = -\frac{\sin(\pi q) e^{at}}{(1+t)^a}.$$

- Franklin-Friedman expansion is expressible in terms of the Laplace-type integral given by

$$\sum_{k=0}^{\infty} c_k(z) \frac{(a)_k}{k! z^{a+k}} = -\frac{\Gamma(b-a)\sin(\pi(b-a-1))}{\pi z^{b-1}} \int_0^\infty \frac{t^{a-b} e^{-zt}}{(1+t)^a} \, dt \, .$$

- Application of Kummer's transformation $U(a,b,z) = z^{1-b} U(1+a-b, 2-b, z)$.

The Franklin-Friedman expansion for $U(a, b, z)$ (computation)

Computation of coefficients $c_k(z)$

- Direct computation
  - Double binomial sum is significantly expensive as k grows $\Longrightarrow$ time complexity $O(N^3)$. ✗
- Recursive algorithm
  - Combine binomial expansion sums to reuse the binomial coefficients, $c_k(z)$ at u_k are computed at once $\Longrightarrow$ time complexity $O(N^2)$. ✓
  - Complete Pascal's triangle until row N can be pre-computed with complexity $O(N^2)$.
  - Optimizations and avoidance of redundant operations.

Proposition

The coefficients $c_k(z)$ of the Franklin-Friedman expansion for the amplitude function $f(t) = (1+t)^{b-a-1}$ satisfy the recurrence equation

$$c_k(z) = u_k + \sum_{i=0}^{k-1} \binom{k}{i} z^{k-i} u_i,$$

where

$$u_k = A_k^{b-a-1-k} k! L_k^{b-a-1-k}(z+a+k) \quad \text{and} \quad c_0 = u_0 = A_0^{b-a-1},$$

$L_k^{\lambda}(z)$ being generalized Laguerre polynomials.

The Franklin-Friedman expansion for $U(a, b, z)$ (experiments (1/4))

Benchmark settings

- Linux Ubuntu
- Intel(R) Core(TM) i7-6700HQ CPU at 2.60GHz.
- Franklin-Friedman, Vanishing saddle point and asymptotic expansion with mpmath 1.0.0.
- Absolute relative errors with Arb evaluated at 5000-10000 bits of precision.

(a, b, z)	N	Asymptotic	Vanishing	Franklin-Friedman
	10	-	3e−14	6e−25
	30	-	7e−34	1e−59
$(600, 600, 500)$	50	-	7e−50	6e−88
	100	-	4e−82	5e−146
	200	-	3e−128	2e−234
	10	-	1e−04	1e−10
	30	-	4e−15	8e−38
$(100, 1, 1000)$	50	4e−02	2e−26	7e−66
	100	1e−27	2e−54	4e−132
	200	9e−60	1e−102	2e−245
	10	-	3e−01	3e−03
	30	-	2e−05	2e−17
$(1000, 500, 5000)$	50	-	1e−11	2e−36
	100	-	2e−31	8e−92
	200	-	4e−78	3e−213

Table: Comparison between various methods for $U(a, b, z)$. Large parameters and argument.

The Franklin-Friedman expansion for $U(a,b,z)$ (experiments (2/4))

(a,b,z)	N	Ascending	Asymptotic	Vanishing	Franklin-Friedman
$(30, 81/4, 300)$	10	-	1e−04	6e−10	8e−20
	30	-	1e−16	8e−26	1e−52
	50	-	1e−27	8e−39	3e−79
	100	-	5e−48	6e−63	5e−131
	200	1e−13 ($N = 1000$)	4e−68	3e−88	4e−202
$(123/4, 101/5, 50)$	10	-	-	8e−04	6e−08
	30	-	-	3e−07	7e−20
	50	-	-	7e−08	2e−28
	100	-	-	-	4e−43
	300	2e−48	-	-	9e−71
$(5/4, 10/4, 30)$	10	-	1e−10	2e−11	8e−19
	30	-	5e−15	4e−16	4e−32
	50	-	7e−13	3e−14	2e−39
	100	6e−11	-	-	4e−50
	200	6e−80	-	-	4e−61
$(401/2, 211/6, 300)$	10	-	-	-	7e−01
	30	-	-	-	1e−04
	50	-	-	-	5e−11
	100	-	-	-	6e−30
	200	4e−53 ($N = 1600$)	-	-	3e−66

Table: Comparison between various methods for $U(a,b,z)$. Small and moderate values of parameters and argument.

The Franklin-Friedman expansion for $U(a, b, z)$ (experiments (3/4))

(a, b, z)	N	Asymptotic	Vanishing	Franklin-Friedman
	10	-	-	-
	30	-	-	-
$(-241/2, 20, 400)$	50	-	-	2e−19
	100	1e−11	3e−16	2e−170
	200	1e−226	4e−138	2e−375
	10	-	-	-
	30	-	-	3e−21
$(-500/6, -21/6, 300)$	50	-	9e−11	2e−87
	100	9e−118	7e−78	9e−212
	200	6e−225	1e−143	3e−334

Table: Comparison between various methods for $U(a, b, z)$. Moderate negative parameters and argument.

The Franklin-Friedman expansion for $U(a, b, z)$ (experiments (4/4))

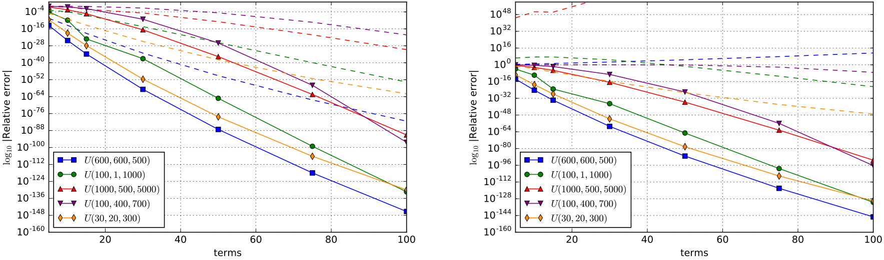


Figure: Compare Franklin-Friedman expansion against vanishing saddle point and asymptotic expansion for fixed number of terms.

Lerch Transcendent

Journal articles

1. G. Navas-Palencia. *Numerical methods and arbitrary-precision computation of the Lerch transcendent*. Preprint 2018, submitted to Numerical Algorithms.

Introduction

- Serves as a unified framework in analytic number theory.
- Applications: theoretical physics (Bose-Einstein condensation distribution, integrals of the Fermi-Dirac distribution), mathematics (Dirichlet *L*-series) and statistics.
- Relevant works: Ferreira et al. (2004), Guillera (2008), Crandall (2012), Paris (2016), ...
- Representations
  - Dirichlet series

$$\Phi(z,s,a)=\sum_{k=0}^{\infty}\frac{z^k}{(k+a)^s},$$

  - Integral representations (Hermite-type and Laplace-type, respectively)

$$\Phi(z,s,a)=\frac{1}{2a^s}+\frac{(-\log(z))^{s-1}}{z^a}\Gamma(1-s,-a\log(z))$$
$$+2\int_0^\infty\frac{\sin(s\arctan(t/a)-t\log(z))}{(a^2+t^2)^{s/2}(e^{2\pi t}-1)}\,dt,\quad \Re(a)>0.$$

$$\Phi(z,s,a)=\frac{1}{\Gamma(s)}\int_0^\infty\frac{t^{s-1}e^{-at}}{1-ze^{-t}}\,dt,\quad \Re(s)>0,\ \Re(a)>0,\ z\notin[1,\infty),$$

Objective

New uniform asymptotic expansions of $\Phi(z,s,a)$ for large order of the parameters a, s and argument z. Special emphasis on the case $\Re(z)\gg 0$.

Euler-MacLaurin formula

Proposition

The Euler-Maclaurin summation formula for the Lerch transcendent is given by

$$\Phi(z, s, a) = S + I + T + R,$$

where

$$S = \sum_{k=0}^{N-1} \frac{z^k}{(k+a)^s},$$

$$I = \frac{(-\log(z))^{s-1}}{z^a} \Gamma(1-s, -(a+N)\log(z)),$$

$$T = \frac{z^N}{(a+N)^s} \left(\frac{1}{2} + \sum_{k=1}^{M} \frac{B_{2k}}{(2k)!} \frac{U(-2k+1, -2k+2-s, -(a+N)\log(z))}{(a+N)^{2k-1}} \right),$$

$$R = -\int_N^\infty \frac{\tilde{B}_{2M}(t)}{(2M)!} \frac{z^t}{(a+t)^{s+2M}} U(-2M, -2M+1-s, -(a+t)\log(z))\, dt,$$

for $a, s, z \in \mathbb{C}$ *with* $|\log(z)| < 2\pi$ *and* $N, M \in \mathbb{N}$ *such that* $\Re(a) + N > 0$ *and* $\Re(s) + 2M > 1$.

Euler-MacLaurin formula (proof sketch)

- Let us first consider the Hermite-type integral

$$I := \int_0^\infty \frac{\sin(s \arctan(t/a) - t \log(z))}{(a^2 + t^2)^{s/2}(e^{2\pi t} - 1)}\, dt\,.$$

For $z, s, a \in \mathbb{R}$, $z > 0$ and $a > 0$, the above integral can be written in the form

$$I = \frac{1}{a^s} \Im \left(\int_0^\infty \frac{z^{-it}}{(1 - it/a)^s} \frac{dt}{e^{2\pi t} - 1} \right).$$

- Express the integrand in terms of the confluent hypergeometric function $U(a, b, z)$

$$I = \frac{1}{a^s} \Im \left((-a \log(z))^s \int_0^\infty \frac{e^{-i \log(t)} U(s, s+1, (it - a) \log(z))}{e^{2\pi t} - 1}\, dt \right).$$

- Apply the addition theorem for $U(a, b, z)$, substitute and interchange summation and integration

$$I = \frac{1}{a^s} \Im \left((-a \log(z))^s \sum_{k=0}^\infty \frac{(-i \log(z))^k U(s, s+k+1, -a \log(z))}{k!} \int_0^\infty \frac{t^k}{e^{2\pi t} - 1}\, dt \right).$$

- Kummer's transformation to rewrite I.
- Finally, taking the imaginary

$$I = \frac{1}{2a^s} \sum_{k=1}^\infty \frac{B_{2k}}{(2k)!} \frac{U(-2k+1, -2k+2-s, -a \log(z))}{a^{2k-1}}.$$

Euler-MacLaurin formula (convergence)

- The expansion is convergent for $|\log(z)| < 2\pi$.
- Take asymptotic estimate of the k-th term

$$
\begin{aligned}
|t_k| &= \left| \frac{B_{2k}}{(2k)!} \frac{U(-2k+1, -2k+2-s, -(a+N)\log(z))}{(a+N)^{2k-1}} \right| \\
&\sim \frac{2}{(2\pi)^{2k}} |\log(z)|^{2k-1}.
\end{aligned}
$$

- Convergence for z the ratio test (d'Alembert ratio test)

$$
\lim_{k\to\infty} \left| \frac{t_{k+1}}{t_k} \right| \sim \frac{|\log(z)^2|}{4\pi^2} < 1 \iff |\log(z)| < 2\pi.
$$

Euler-MacLaurin formula (rigorous error bound + proof sketch)

Theorem (G. Navas-Palencia, 2018)

Given $a, s, z \in \mathbb{C}$ with $|\log(z)| < 2\pi$ and $N, M \in \mathbb{N}$ such that $\Re(a) + N > 0$ and $\Re(s) + 2M > 1$, the error term in the Euler-Maclaurin summation formula satisfies

$$|R| \leq \frac{4}{(2\pi)^{2M}} \left| C \sum_{k=0}^{2M} \binom{2M}{k} Q(k+1-2M-s, W) \frac{(-\log(z))^{-k-1+2M+s}}{\log^{-k}(z)} \right|,$$

where $C = \Gamma(1-s)/z^a$, $W = -(a+N)\log(z)$ and $Q(a,z) = \Gamma(a,z)/\Gamma(a)$ is the regularized incomplete Gamma function.

- Ideas of the proof
  - upper bound for $|\tilde{B}_n(t)| < 4n!/(2\pi)^n$.
  - interchange integration and the expansion of $U(-2M, -2M+1-s, -(a+N)\log(z))$.
  - resulting integral expressible in terms of the incomplete Gamma function $\Gamma(a,z)$.

Uniform asymptotic expansion

- Vanishing saddle-point method to the Laplace-type integral representation.
- Expansion in terms of Eulerian polynomials $A_k(z)$ and Tricomi-Carlitz polynomials $P_k(\lambda)$.
- Extension domain of the Poincaré type asymptotic expansion for large a (Ferreira, 2004).
  - Uniform asymptotic expansion for large a, s and z. ✓
  - Large values of $\Re(s)$ and $|z|$ improve the asymptotic convergence of the expansion.

Proposition

For $a, s, z \in \mathbb{C}$, $\Re(a) > 0$ and $z \notin [1, \infty)$ we have the following uniform asymptotic expansion for $\Phi(z, s, a)$

$$\Phi(z,s,a) = \frac{e^{\mu}}{e^{\mu} - z}\left(\frac{1}{a^s} + \sum_{k=2}^{K-1}(-1)^k \frac{P_k(s)}{k!\,a^{k+s}} r^k A_k\left(\frac{e^{\mu}}{z}\right)\right) + \varepsilon_K(z,s,a),$$

where $r = z/(e^{\mu} - z)$.

- Rigorous error bound by comparison with a geometric series.
- Saddle point bounds for polynomials $P_k(z)$ and $A_k(z)$.

Asymptotic expansion for large z

Theorem (G. Navas-Palencia, 2018)

For $a, s, z \in \mathbb{C}$ and $\Re(a) > 0$ we have an asymptotic expansion for large a and z, and fixed s given by

$$\Phi(z,s,a) \sim \frac{1}{2a^s} + \frac{(-\log(z))^{s-1}}{z^a}\Gamma(1-s,-a\log(z))$$
$$+ \frac{1}{2a^s}\left(\frac{2}{\log(z)} - \coth\left(\frac{\log(z)}{2}\right)\right)$$
$$+ \frac{1}{a^s}\sum_{k=1}^{\infty}\frac{(s)_k}{a^k(2\pi)^{k+1}}\left(\frac{1}{u^{k+1}} - \frac{\pi^{k+1}}{k!}\coth(\pi u)^{k-1}\operatorname{csch}(\pi u)^2\mathcal{P}_k(\operatorname{sech}(\pi u)^2)\right),$$

where $u = \frac{\log(z)}{2\pi}$ and $\mathcal{P}_k(x)$ are peak polynomials.

Asymptotic expansion for large z (proof sketch)

- Application of the binomial theorem yields

$$I = \Im\left(\int_0^\infty \frac{z^{-it}}{(1-it/a)^s}\frac{dt}{e^{2\pi t}-1}\right) = \Im\left(\sum_{k=0}^\infty \frac{(s)_k}{k!}\left(\frac{i}{a}\right)^k \int_0^\infty \frac{z^{-it}t^k}{e^{2\pi t}-1}\,dt\right).$$

$$I_k = \int_0^\infty \frac{z^{-it}t^k}{e^{2\pi t}-1}\,dt = \int_0^\infty \frac{z^{-it}t^k(1-e^{-t})}{(1-e^{-t})(e^{2\pi t}-1)}\,dt = \frac{k!}{(2\pi)^{k+1}}\zeta\left(k+1, 1+i\frac{\log(z)}{2\pi}\right).$$

$$I \sim \frac{1}{4}\left(\frac{2}{\log(z)} - \coth\left(\frac{\log(z)}{2}\right)\right) + \sum_{k=1}^\infty \frac{(s)_k}{a^k(2\pi)^{k+1}}\Im\left(i^k\zeta\left(k+1, 1+i\frac{\log(z)}{2\pi}\right)\right).$$

- Hereinafter we use $u = \frac{\log(z)}{2\pi}$ to simplify notation. Let us define the terms $C_k(u)$ as

$$C_k(u) = \Im\left(i^k\zeta\left(k+1, 1+iu\right)\right) = \frac{i^{k+1}}{2}\left((-1)^k\zeta\left(k+1, 1-iu\right) - \zeta\left(k+1, 1+iu\right)\right),$$

- The first five coefficients $c_k(u) = 2C_k(u)$ are

$$C_k(u) = \frac{1}{2u^{k+1}} - \frac{\pi^{k+1}}{2k!}\coth(\pi u)^{k-1}\operatorname{csch}(\pi u)^2\mathcal{P}_k(\operatorname{sech}(\pi u)^2).$$

where $\mathcal{P}_k(x)$ are *pk-polynomial*.

Algorithmic details (Euler-MacLaurin formula - Tail)

- Estimation of number of terms M for P-bit precision

$$M \sim \left[\frac{1}{2} \left| \frac{\log(2^{-P-1}\log(z))}{\log(2\pi) - \log(\log(z))} \right| \right].$$

- Evaluation of the tail

$$T = \frac{z^N}{(a+N)^s} \left(\frac{1}{2} + \sum_{k=1}^{M} \frac{B_{2k}}{(2k)!} (-\log(z))^{2k-1} T_2^{(k)} \right).$$

Terms $T_2^{(k)}$ can be constructed using a linear holonomic recurrence equation

$$p = s - (a+N)\log(z)), \quad q = -\frac{1}{(a+N)\log(z)}.$$

The sequence of terms $T_2^{(k)}$ satisfy the recurrence equation

$$T_1^{(k)} = [pT_2^{(k-1)} + (2k-3)(T_2^{(k-1)} - T_1^{(k-1)})]q, \quad T_2^{(k)} = [pT_1^{(k)} + (2k-2)(T_1^{(k)} - T_2^{(k-1)})]q$$

for $k \geq 2$, with initial values $T_1^{(1)} = 1$ and $T_2^{(1)} = 1 - \frac{s}{(a+N)\log(z)}$.

Algorithmic details (Asymptotic expansions)

- Drawback: computing a large number of Eulerian and peak polynomials efficiently.
- Computing the first k Eulerian polynomials simultaneously recursively. Given $A_0(z), \ldots, A_{k-1}(z)$, compute $A_k(z)$ in $\mathcal{O}(k)$ arithmetic operations.
  - $A_k(z)$ has $\mathcal{O}(k \log k)$ bits, the algorithm needs $\mathcal{O}(k^{3+o(1)})$ bit operations and $\mathcal{O}(k^2 \log k)$ space.
  - Compute $A_0(2), \ldots, A_{1000}(2)$ at 333-bit precision in 1.51 seconds on a 2.6 GHz Intel i7 processor.
  - Improvements: recycle terms of the sum of Eulerian polynomial series and binary exponentiation when j is prime and multiplication otherwise.
- Use Mittag-Leffler type decomposition asymptotic series for large degree k.
- Peak polynomials using generating function for peak numbers.
  - Computing the triangular array for the first 1000 peak numbers using recurrence takes 1.55 seconds.
  - For larger k the functional relation with the Eulerian polynomial.
- Accurate estimate of optimal truncation level + refinement via linear search.

Benchmarking (1/3)

Benchmark settings

- Linux Ubuntu
- Intel(R) Core(TM) i7-6700HQ CPU at 2.60GHz. 4 cores for parallel mode.
- Mathematica 10.4 and mpmath 1.0.0. Both GMP library.
- Implementation using mpmath 1.0.0.

$\Phi(z, s, a)$	bits	Mathematica	L-series	Parallel	Euler-Maclaurin
	64	0.0011	0.0011	-	-
$z = 1/4$	333	0.0067	0.0055	-	-
$s = 10/4$	1024	0.0339	0.0155	-	-
$a = 20/7$	3333	0.7313	0.0660	0.0431	-
	10000	21.406	0.4885	0.1513	-
	64	0.0015	0.0069	-	0.0031 (0.0053)
$z = 9/10$	333	0.0109	0.0607	0.0429	0.0153 (0.0255)
$s = 10/4$	1024	0.0984	0.2165	0.1052	0.0166 (0.0222)
$a = 20/7$	3333	1.8843	1.0422	0.3281	0.0953 (0.1197)
	10000	39.937	8.6969	2.4881	2.7331 (3.1578)
	64	0.0031	0.0020	-	-
$z = -6/10$	333	0.0156	0.0083	-	-
$s = 10/4$	1024	0.1422	0.0243	-	-
$a = 20/7$	3333	3.0922	0.0983	-	-
	10000	21.2969	0.7500	-	-

Table: Time (in seconds) to compute $\Phi(z, s, a)$ for small argument $|z|$.

Benchmarking (2/3)

$\Phi(z, s, a)$	bits	mpmath	Mathematica	Euler-Maclaurin	Parallel
	64	0.096 (0.139)	0.313	0.008 (0.013)	-
$z = 2.5 + 1.5i$	333	1.09 (1.21)	0.672	0.041 (0.089)	-
$s = 1.25 + 2i$	1024	8.39 (9.38)	3.14	0.128 (0.233)	-
$a = 3.5 + 5i$	3333	154.4 (161.1)	27	1.64 (2.37)	-
	10000	1564.6	438	25.04 (33.33)	19.06 (27.32)
	64	0.263 (0.295)	0.047	0.016 (0.039)	-
$z = 2.5 + 7.5i$	333	1.79 (1.98)	0.250	0.110 (0.250)	-
$s = -50.25 + 10i$	1024	6.59 (7.05)	1.58	0.72 (1.49)	-
$a = 1.5 - i$	3333	133.6 (135.1)	21.66	11.83 (16.64)	8.72 (13.22)
	10000	1453	409.1	190.3 (224.5)	153.2 (196.5)
	64	0.253 (0.324)	0.031	0.013 (0.022)	-
$z = 2.5 + 0.5i$	333	1.79 (1.92)	0.265	0.058 (0.104)	-
$s = -100.25 + 10i$	1024	12.66 (13.94)	7.72	0.298 (0.685)	-
$a = 100.5 - 10i$	3333	120.7 (127.1)	83.14	2.97 (4.19)	-
	10000	1500.6	> 1800	24.65 (32.89)	18.88 (28.34)

Table: Time (in seconds) to compute $\Phi(z, s, a)$ with moderate values of z, s and a to 64, 333, 1024, 3333 and 10000 bits of precision. First evaluation pre-computing Bernoulli numbers within parentheses. Maximum time 1800 seconds.

Benchmarking (3/3)

$\Phi(z,s,a)$	bits	mpmath	Mathematica	Euler-Maclaurin	Asymptotic	K	peak time
$z = 140$	64	0.0684	0.0154	0.0027	0.0022	9	6.3%
$s = 1/4$	333	0.7859	0.1219	2.2342	0.0134	59	10.9%
$a = 200$	1024	5.0361	0.7297	-	0.1931	254	10.5%
	64	0.1238	0.0661	-	0.0017	6	4.6%
$z = 10000$	333	1.5456	0.2078	-	0.0066	34	11.5%
$s = 10/4$	1024	9.9478	1.0406	-	0.0481	122	10.0%
$a = 2000$	3333	94.362	15.141	-	0.9498	493	8.4%
	10000	1978.2	283.21	-	39.779	1952	6.0%

Table: Time (in seconds) to compute $\Phi(z,s,a)$ for large parameter a and argument z. Comparison to Euler-Maclaurin at low precision. The rightmost column shows the percentage of the total time devoted to computation of K peak numbers.

$\Phi(z,s,a)$	bits	mpmath	Mathematica	Asymptotic	Uniform	Eulerian time
$z = -200.65$	64	0.0228*	0.0469	0.0031 (16)	0.0173 (20)	97.0%
$s = 100.25$	333	0.0149*	0.1563	0.0412 (104)	0.0592 (60)	97.5%
$a = 501.5$	1024	1.0219**	0.8438	0.7512 (421)	0.5151 (229)	98.8%
$z = -20000$	64	0.0101*	0.0312	0.0027 (15)	0.0051 (9)	93.2%
$s = 100.25$	333	0.0168*	0.1875	0.0362 (93)	0.0436 (53)	96.9%
$a = 501.5$	1024	1.7736	1.0313	0.5424 (365)	0.2964 (196)	98.3%

Table: Time (in seconds) to compute $\Phi(z,s,a)$ for large parameter a and s, and argument z. Number of terms for each expansion within parentheses. For mpmath: (*) and (**) indicate no answer and inaccurate answer, respectively.

Thank you!