Numerics of Special Functions

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Literature

Literature, Methods and Software

- Maple, Mathematica, Matlab, Macsyma
- Collections of algorithms: NAG, IMSL, SLATEC, CERN
- Published algorithms: ACM, CPC, Applied Statistics
- Repositories: GAMS at NIST, Netlib
Some simple experiences

- How to compute an integral?
- Another integral
- Exponential integral: $\text{Ei}(x)$ or $\text{Ei}(z)$?
- Take a special case
- Scaling
- Extra elementary functions
- Example: Beta integral
- Example: Confluent hypergeometric function
How to compute an integral?

Consider

\[ F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda\sqrt{t^2+1}} \, dt. \]

Maple 7, for \( \lambda = 10 \), gives

\[ F(10) = -0.1837516481 + 0.5305342893i. \]
How to compute an integral?

Consider

\[ F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda \sqrt{t^2+1}} dt. \]

Maple 7, for \( \lambda = 10 \), gives

\[ F(10) = -0.1837516481 + 0.5305342893i. \]

With Digits = 40, the answer is

\[ F(10) = -0.1837516480532069664418890663053408790017 + 0.5305342892550606876095028928250448740020i. \]
Take another integral, which is almost the same:

\[ F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2 + 2i\lambda \sqrt{t^2 + 1}} \, dt \quad \Rightarrow \quad G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2 + 2i\lambda t} \, dt. \]

Maple 7, for \( \lambda = 10 \), gives \( G(10) = -0.1387778781 \times 10^{-15} \).
Take another integral, which is almost the same:

\[
F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda\sqrt{t^2+1}} dt \quad \implies \quad G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda t} dt.
\]

- Maple 7, for \( \lambda = 10 \), gives \( G(10) = -0.1387778781 \times 10^{-15} \).
- With Digits = 40, the answer is \( G(10) = 0.16 \times 10^{-42} \).
Take another integral, which is almost the same:

\[ F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda\sqrt{t^2+1}} \, dt \quad \implies \quad G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda t} \, dt. \]

- Maple 7, for \( \lambda = 10 \), gives \( G(10) = -0.1387778781 \times 10^{-15} \).
- With Digits = 40, the answer is \( G(10) = 0.16 \times 10^{-42} \).
- The correct answer is \( G(\lambda) = \sqrt{\pi}e^{-\lambda^2} \) and for \( \lambda = 10 \) we have \( G(10) = 0.6593662989 \times 10^{-43} \).
The message is: one should have some feeling about the computed result.

Otherwise a completely incorrect answer can be accepted.

Mathematica is more reliable here, and says:

"NIntegrate failed to converge to prescribed accuracy after 7 recursive bisections in $t$ near $t = 2.9384615384615387$".
By the way, ask Maple 7 to do the following integral

\[ H(\lambda) = \int_{-\infty}^{\infty} e^{-t^2 + 2i\lambda \sqrt{t^2}} \, dt, \]

and the funny answer is, after some simplification,

\[ H(\lambda) = \sqrt{\pi} e^{-\lambda^2} \left[ 1 + \text{signum}(t) \, \text{erf} \, i\lambda \right], \]

where \( \text{erf} \, z \) is the error function.
Another integral

Consider

\[ F(u) = \int_{0}^{\infty} e^{uit} \frac{dt}{t - 1 - i}, \quad u > 0. \]

Numerical quadrature gives \( F(2) = -0.934349 - 0.70922i \).

Mathematica 4.1 gives for \( u = 2 \) in terms of the Meijer G-function:

\[
F(2) = \pi G^{2,1}_{2,3} \left( \begin{array}{c}
0, \frac{1}{2} \\
0, 0, \frac{1}{2}
\end{array} ; 2 - 2i \right) .
\]

Mathematica evaluates: \( F(2) = -0.547745 - 0.532287i \).
Ask Mathematica to evaluate $F(u)$:

$$F(u) = e^{iu} - u \Gamma(0, iu - u).$$

This gives $F(2) = -0.16114 - 0.355355i$.

So, we have three numerical results:

$$F_1 = -0.934349 - 0.70922i,$$

$$F_2 = -0.547745 - 0.532287i,$$

$$F_3 = -0.16114 - 0.355355i.$$

Observe that $F_2 = (F_1 + F_3)/2$. $F_1$ is correct.
Maple:

\[ F(u) = e^{iu-u} \text{Ei}(1, iu - u) = e^{iu-u} \Gamma(0, iu - u) \]

same as Mathematica. This is a wrong answer.

Next, Maple, after simplification, in terms of exponential integrals:

\[ F(2) = e^{2i-2} \text{Ei}(1, 2i - 2) + 2\pi i e^{2i-2} \]

giving \[ F(2) = -0.9343493870 - 0.7092195099i \], which is the correct answer.
The exponential integrals are defined by

\[ E_1(z) = \int_{z}^{\infty} \frac{e^{-t}}{t} \, dt, \quad |\text{ph} \, z| < \pi, \quad \text{Ei}(x) = -\int_{-\infty}^{x} \frac{e^{-t}}{t} \, dt = \int_{-\infty}^{x} \frac{e^t}{t} \, dt, \quad x > 0, \]

\[ \text{Ei}(x) = -\int_{-x}^{\infty} \frac{e^{-t}}{t} \, dt = -E_1(-x), \quad x < 0. \]

Maple requires real \( x \) in \( \text{Ei}(x) \), as is in agreement with this definition.

Mathematica accepts complex \( z \) in \( \text{Ei}(z) \), although The Mathematica Book (4th Ed., p. 765) defines \( \text{Ei}(z) \) only for \( z > 0 \) by using a principal value integral. This is confusing.

The same happens in Gradshteyn & Ryzhik (Sixth Ed.): \( \text{Ei}(x) \) is only defined as above; there is no proper definition of the exponential integral for complex argument.
Take a special case

Parabolic cylinder functions are special cases of the $_1F_1$ functions, Kummer functions or Whittaker functions. The Mathematica Book (4th Ed., p. 765) advises to use

\[ U(a, z) = 2^{-a/2} z^{-1/2} W_{-a/2, -1/4} \left( \frac{1}{2} z^2 \right), \]

but this is useless when \( z < 0 \).

Maple 7 uses the representations in terms of $_1F_1$ functions, but this becomes very unstable when the parameters are "large".
Scaling

The function $\Gamma^*(z)$ defined by

$$\Gamma(z) = \sqrt{2\pi} z^{z-1/2} e^{-z} \Gamma^*(z),$$

$$\Gamma^*(z) \sim 1 + \frac{1}{12z} + \frac{1}{288z^2} + \ldots , \quad z \to \infty,$$

can be computed within machine precision for almost all complex $z$. The precision in the gamma function itself follows from the evaluation of the elementary function

$$\sqrt{2\pi} z^{z-1/2} e^{-z}.$$

To avoid underflow and overflow, and to control accuracy, it is very important to have scaled functions like $\Gamma^*(z)$ available.
The same holds for Bessel functions, parabolic cylinder functions, and so on.

The scaled Airy function $\widetilde{\text{Ai}}(z)$ defined by

$$\text{Ai}(z) = e^{-\frac{2}{3}z^{3/2}} \widetilde{\text{Ai}}(z)$$

can be computed very accurate for complex $z$ (not close to zeros of $\text{Ai}(z)$).

The scaling factor $e^{-\frac{2}{3}z^{3/2}}$ completely determines the accuracy if $z$ is large and complex.

Again, scaled functions are very useful to avoid underflow and overflow, and to control accuracy.
We have standard codes for

\[
\sin x, \quad \ln x, \quad \arctan x, \quad e^x, \ldots
\]

but usually not for

\[
\frac{\sin x - x}{x^3}, \quad \frac{\ln(1 + x)}{x}, \quad \frac{\arctan x - x}{x^3}, \quad \frac{e^x - 1}{x}, \ldots
\]

for small values of \( x \). It is not difficult to write efficient codes (by using power series, for example). A standard package for this type of elementary functions would be very useful.
Example: Beta integral

The Beta integral can be written in the form

\[
\frac{\Gamma(p)\Gamma(q)}{\Gamma(p + q)} = \sqrt{2\pi} \sqrt{\frac{p + q}{pq}} \frac{\Gamma^*(p)\Gamma^*(q)}{\Gamma^*(p + q)} e^{p \ln(1 - \frac{q}{p + q}) + q \ln(1 - \frac{p}{p + q})}.
\]

When \( p + q \) is large, all quantities at the right-hand side can be computed in good relative precision if codes for \( \ln(1 + x) \) (for small \( x \)) and \( \Gamma^*(x) \) (for large \( x \)) are available.
Example: Confluent hypergeometric function

The standard solution of Kummer’s equation that is singular at the origin can be written in the form

\[
U(a, c, z) = \frac{\pi}{\sin \pi c} \left[ \frac{1 F_1(a; c; z)}{\Gamma(1 + a - c) \Gamma(c)} - z^{1-c} \frac{1 F_1(1 + a - c; 2 - c; z)}{\Gamma(a) \Gamma(2 - c)} \right].
\]

For small \( z \) this can be used for computations.

However, for integer values of \( c \), problems arise.

A careful analysis is needed to avoid numerical cancellations.
We have

\[ U(a, c, z) = \sum_{k=0}^{\infty} f_k x^k, \]

where

\[ f_0 = \frac{\pi}{\sin \pi c} \frac{1}{\Gamma(1 + a - c) \Gamma(c)} = \frac{\Gamma(1 - c)}{\Gamma(1 + a - c)}, \]

and

\[ f_1 = \frac{\pi}{\sin \pi c} \left[ \frac{a}{\Gamma(1 + c) \Gamma(1 + a - c)} - \frac{z^{-c}}{\Gamma(a) \Gamma(2 - c)} \right]. \]

For small values of \( c \) the coefficient \( f_1 \) is difficult to compute.
An expansion in powers of $c$ is not doable, because of all higher derivatives of the gamma function.

The computation of $f_1$ can be done if we have an algorithm for

$$
\frac{1}{\beta} \left[ \frac{1}{\Gamma(\alpha - \beta)} - \frac{1}{\Gamma(\alpha + \beta)} \right], \quad \text{or} \quad \frac{1}{\beta} \left[ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha - \beta)} - 1 \right]
$$

for small values of $|\beta|$, $\alpha \in \mathbb{C}$.

The remaining $f_k$ can be obtained from recursions, if $f_1$ is available.
Numerical aspects

- Fixed precision or variable precision
- Insight in function behavior
- Selecting analytical tools
- Selecting numerical methods
- Stability of the algorithms
- Efficiency of the algorithms
- Underflow, overflow, scaling
- Testing
- High quality software
Fixed precision or variable precision

- Fixed precision: efficiency
- Variable precision: greater challenge
Insight in function behavior

- Numerically satisfactory pair of solutions
- Singular points, turning points
- Influence of additional parameters
- Stable representations
Selecting analytical tools

- Are power series available?
- Are asymptotic expansions available?
- Are these uniform with respect to parameters?
- Are new expansions needed?
- Are integrals well conditioned?
- Are connection formulas available?
Selecting numerical methods

- Power series: convergent, asymptotic
- Recursions, linear difference equations
- Chebyshev expansions
- Continued fractions
- Quadrature: Gauss, trapezoidal
- Uniform asymptotic expansions
- Differential equations
- Rational approximations, Padé, Chebyshev sense
- Convergence acceleration
Stability of the algorithms

- Rigorous error analysis?
- Connection formulas
- An important source of errors: elementary functions with large complex arguments
Efficiency of the algorithms

- One universal algorithm?
- Power series if possible?
Underflow, overflow, scaling

- Avoid underflow or overflow by scaling
- Discontinuous scaling factors may occur
- Testing scaled functions: no guarantee
Testing

- Wronskian relations
- Contiguous relations
- Other functional identities
- Testing by using overlapping domains
- Testing with multiple-precision algorithms
- Comparison against a standard
- Lozier (1996) Test service and reference software
High quality software

- Refereed articles
- Refereed software
- Concern: maintenance
Numerical methods

- Power series: convergent, asymptotic
- Recursions, linear difference equations
- Chebyshev expansions
- Continued fractions
- Quadrature, Gauss, trapezoidal
- Uniform asymptotic expansions
- Differential equations
- Rational approximations, Padé, Chebyshev sense
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Power series: convergent, asymptotic

- Estimating remainders
- "Convergence" of asymptotic expansions
- Domains: Where to use the series?
- Meaning of asymptotic expansions
Meaning of asymptotic expansions

Consider the expansion of the Kummer function:

\[
\frac{1}{\Gamma(c)} \binom{\frac{1}{c} \left( a, c, z \right)}{\frac{1}{\Gamma(a)}} = e^z z^{a-c} \left[ \sum_{n=0}^{R-1} \frac{(c-a)_n(1-a)_n}{n! z^n} + \mathcal{O} \left( |z|^{-R} \right) \right] +
\]

\[
\frac{z^{-a}}{\Gamma(c-a)} \left[ \sum_{n=0}^{S-1} \frac{(-1)^n(a)_n(1+a-c)_n}{n! z^n} + \mathcal{O} \left( |z|^{-S} \right) \right] e^{\pm i\pi a},
\]

This expansion is valid for large complex \( z \) in certain sectors, but also for positive \( z \).
Meaning of asymptotic expansions

Consider the expansion of the Kummer function:

\[
\frac{1F_1(a; c; z)}{\Gamma(c)} = \frac{e^z z^{a-c}}{\Gamma(a)} \left[ \sum_{n=0}^{R-1} \frac{(c-a)_n (1-a)_n}{n! z^n} + \mathcal{O}\left(|z|^{-R}\right) \right] +
\]

\[
\frac{z^{-a}}{\Gamma(c-a)} \left[ \sum_{n=0}^{S-1} \frac{(-1)^n (a)_n (1+a-c)_n}{n! z^n} + \mathcal{O}\left(|z|^{-S}\right) \right] e^{\pm i\pi a}
\]

This expansion is valid for large complex \( z \) in certain sectors, but also for positive \( z \).
Observe that \( e^{\pm i\pi a} \) is a complex quantity.
Meaning of asymptotic expansions

Consider the expansion of the Kummer function:

\[
\frac{1}{\Gamma(c)} \frac{1 F_1(a; c; z)}{\Gamma(a)} = e^z z^{a-c} \Gamma(a) \left[ \sum_{n=0}^{R-1} \frac{(c-a)_n(1-a)_n}{n! z^n} + O \left( |z|^{-R} \right) \right] + \\
\frac{z^{-a}}{\Gamma(c-a)} \left[ \sum_{n=0}^{S-1} (-1)^n \frac{(a)_n(1+a-c)_n}{n! z^n} + O \left( |z|^{-S} \right) \right] e^{\pm i\pi a}
\]

This expansion is valid for large complex \( z \) in certain sectors, but also for positive \( z \).

Observe that \( e^{\pm i\pi a} \) is a complex quantity.

If \( z > 0 \), \( a \) and \( c \) are real: Does this formula give a complex approximation of a real function?
Recursions, linear difference equations

- First and second order difference equations
- Stability analysis
- Backward recursion
- Nonlinear recursions: Gauss, Landen, AGM
Chebyshev expansions

- Clenshaw, Luke: one variable, tabled coefficients
- Luke: hypergeometric functions

\[
(\omega z)^a U(a, c, \omega z) = \sum_{n=0}^{\infty} C_n(z) T_n^*(1/\omega),
\]

where \( T_n^* \) is the shifted Chebyshev polynomial, \( 1 \leq \omega \leq \infty \), \( z \neq 0, |\text{ph} \ z| < 3\pi/2 \).

The coefficients \( C_n(z) \) are known as Meijer’s G function, and \( C_n(z) \) satisfy a third order linear difference equation.

If \( |\text{ph} \ z| < \pi \) the \( C_n(z) \) can be computed by using a backward recursion scheme.
Continued fractions

- Upper and lower approximations
- Transformations
- Stopping criterion
- Anomalous convergence (Gautschi (1977))
Quadrature, Gauss, trapezoidal

- Gauss quadrature: for fixed precision
- Trapezoidal rule: more flexible
- Select suitable contours: avoid strong oscillations

\[ G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2 + 2i\lambda t} \, dt = e^{-\lambda^2} \int_{-\infty}^{\infty} e^{-s^2} \, ds. \]
Uniform asymptotic expansions

- Computation of coefficients
- Domains: Where to use the expansions?
- Main approximants: higher transcendentals

For example, the Airy-type expansion for the $J$ Bessel function: as $\nu \to \infty$

$$J_\nu(\nu z) \sim \phi(\zeta) \left[ \frac{\text{Ai}(\nu^{2/3}\zeta)}{\nu^{1/3}} \sum_{s=0}^{\infty} \frac{A_s(\zeta)}{\nu^{2s}} + \frac{\text{Ai}'(\nu^{2/3}\zeta)}{\nu^{5/3}} \sum_{s=0}^{\infty} \frac{B_s(\zeta)}{\nu^{2s}} \right],$$

$$\phi(\zeta) = \left( \frac{4\zeta}{1 - z^2} \right)^{1/4}, \quad \frac{2}{3} \zeta^{3/2} = \ln \frac{1 + \sqrt{1 - z^2}}{z} - \sqrt{1 - z^2}.$$
Differential equations

- Stability
- Direction of integration
- Parallel integration (Lozier & Olver (1993))
- Higher order linear equations
- Lanczos $\tau$—method (Coleman, Rappoport)
Rational approximations, Padé, Chebyshev sense

- Cody and co-workers: one variable rational approximations
- Padé: applicable when coefficients can be obtained easily
- Luke: tabled coefficients
Convergence acceleration

- Summing slowly convergent series
- Summing divergent asymptotic series
- Brezinski, Weniger
- Special examples show impressive results
New approaches

- Elementary functions: rigorous bounds
- Multiple-precision computations
- Unrestricted algorithms, error analysis
- Methods for computing symmetric integrals
- New packages for special functions
Elementary functions: rigorous bounds

- Cody & Waite (1980)
- Table-lookup algorithms ((Tang (1991), Rump (2001))
- Zimmerman (France): The MPFR library (www.mpfr.org)
- Cuyt & Verdonk (Belgium): continued fraction approach
Multiple-precision computations

- Brent (1978): Fortran
- Several packages in C, C++
- Maple, Mathematica, ...

Numerics of Special Functions, IMA, Special Functions in the Digital Age, July 2002 – p.45/65
Methods for computing symmetric integrals

Main application: elliptic integrals. Carlson’s method: To iterate the duplication theorem and then sum a five degree power series.

The symmetric integrals are of the form:

$$R_F(x, y, z) = \frac{1}{2} \int_0^\infty \left[ (t + x)(t + y)(t + z) \right]^{-1/2} dt,$$

$$R_J(x, y, z) = \frac{3}{2} \int_0^\infty \left[ (t + x)(t + y)(t + z) \right]^{-1/2} (t + p)^{-1} dt,$$

The algorithms are very efficient and reliable.
New packages for special functions

- Gautschi (1994): ORTHOPOL, also for Gauss-type quadrature rules
- Koepf (1999): orthogonal polynomials, hypergeometric functions (numerics and symbolic)
- Zeilberger (1990, ...) (and others): hypergeometric identities
Why is new software needed?

Are other software efforts still needed with the libraries of Mathematica and Maple available?

A few remarks:
- Refereed software
- Repositories of free software
- Fast algorithms in Fortran77, Fortran90, C, C++
What has to be done?

- Reliable software for large parameter cases
- Appropriate scaling to avoid underflow and overflow
- Complex variables
- The land beyond Bessel
- Integrals of special functions
- $q$– special functions?
Present project

(In collaboration with Amparo Gil and Javier Segura, Madrid).

- Airy functions
- Scorer functions
- $K_{ia}(x), R I_{ia}(x), x > 0, a \in \mathbb{R}$
- Parabolic cylinder functions for real arguments
- Main tool: quadrature of integrals on complex contours, with saddle point analysis
Quadrature of integrals

A simple example is:

\[ G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2 + 2i\lambda t} \, dt = e^{-\lambda^2} \int_{-\infty}^{\infty} e^{-s^2} \, ds. \]

This makes sense, because

- The new integral is real, without oscillations
- The dominant term \( e^{-\lambda^2} \) is in front of the new integral
The function $K_{ia}(x)$

An integral representation:

$$K_{ia}(x) = \int_{-\infty}^{\infty} e^{-x \cosh w + iaw} \, dw.$$ 

Consider the case $0 \leq a < x$ for which values $K_{ia}(x) > 0$, although strong oscillations occur in the integral when $a, x$ are both large. Deform the contour such that no oscillations occur. Write $w = u + iv$; we have

$$-x \cosh w + iaw = -x \cosh u \cos v - av + i(-x \sinh u \sin v + au).$$

Take the imaginary part equal to zero.
This happens when, see the figure,

\[ v = \arcsin \left( \frac{a}{x \sinh u} \cdot \frac{u}{x} \right). \]

The contour runs through the saddle point at

\[ v_0 = \arcsin \left( \frac{a}{x} \right). \]
Integrate along this contour. Then, for $0 \leq a < x$, 

$$K_{ia}(x) = \int_{-\infty}^{\infty} e^{-\phi(u)} f(u) \, du = e^{-\phi(0)} \int_{-\infty}^{\infty} e^{-[\phi(u)-\phi(0)]} \, du$$

where 

$$\phi(u) = x \cosh u \cos v + av, \quad \phi(0) = \sqrt{x^2 - a^2} + a \arcsin(a/x),$$

and $f(u) = \frac{dw}{du} = 1 + i \frac{dv}{du}$.

The function $\phi(u)$ is positive. The factor $e^{-\phi(0)}$ gives the dominant term in the asymptotic behaviour.
Trapezoidal rule

\[ \int_{a}^{b} f(t) \, dt = \frac{1}{2} h[f(a) + f(b)] + h \sum_{j=1}^{n-1} f(hj) + R_n, \quad h = \frac{b - a}{n}. \]

Compared with Gauss quadrature: very flexible; precomputed zeros and weights are not needed.
Trapezoidal rule

\[ \int_a^b f(t) \, dt = \frac{1}{2} h[f(a) + f(b)] + h \sum_{j=1}^{n-1} f(hj) + R_n, \quad h = \frac{b - a}{n}. \]

- Compared with Gauss quadrature: very flexible; precomputed zeros and weights are not needed.
- Error term, for some \( \xi \in (a, b) \):

\[ R_n = -\frac{n h^3}{12} f''(\xi). \]
Trapezoidal rule

\[ \int_a^b f(t) \, dt = \frac{1}{2} h [f(a) + f(b)] + h \sum_{j=1}^{n-1} f(hj) + R_n, \quad h = \frac{b - a}{n}. \]

- Compared with Gauss quadrature: very flexible; precomputed zeros and weights are not needed.
- Error term, for some \( \xi \in (a, b) \):

\[ R_n = - \frac{n}{12} h^3 f''(\xi). \]

- Adaptive algorithm: use previous function values \((h \rightarrow h/2)\).
Example: fast convergence

Take as an example the Bessel function \((h = \pi/n, x = 5)\)

\[
\pi J_0(x) = \int_0^\pi \cos(x \sin t) \, dt = h + h \sum_{j=1}^{n-1} \cos [x \sin(h j)] + R_n,
\]

<table>
<thead>
<tr>
<th>(n)</th>
<th>(R_n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>(-.12 \times 10^{-0})</td>
</tr>
<tr>
<td>8</td>
<td>(-.48 \times 10^{-6})</td>
</tr>
<tr>
<td>16</td>
<td>(-.11 \times 10^{-21})</td>
</tr>
<tr>
<td>32</td>
<td>(-.13 \times 10^{-62})</td>
</tr>
<tr>
<td>64</td>
<td>(-.13 \times 10^{-163})</td>
</tr>
<tr>
<td>128</td>
<td>(-.53 \times 10^{-404})</td>
</tr>
</tbody>
</table>

Much better than the estimate of \(R_n\). Explanation: periodicity and smoothness.
The remainder: smooth and periodic

In fact we have

**Theorem**

If $f(t)$ is periodic and has a continuous $k^{th}$ derivative, and if the integral is taken over a period, then

$$|R_n| \leq \frac{\text{constant}}{n^k}.$$  

Bessel function: we can take any $k$.


$$|R_n| \leq 2e^{x/2} \frac{(x/2)^{2n}}{(2n)!},$$

which is quite realistic for the value of $x$ we chose.
The trapezoidal rule on $\mathbb{R}$

For integrals over $\mathbb{R}$ the trapezoidal rule may again be very efficient and accurate. Consider

$$\int_{-\infty}^{\infty} f(t) \, dt = h \sum_{j=-\infty}^{\infty} f(hj + d) + R_d(h)$$

where $h > 0$ and $0 \leq d < h$.

We use this for functions analytic in the strip:

$$G_a = \{ z = x + iy \mid x \in \mathbb{R}, \ -a < y < a \}.$$
A class of analytic functions

Let $H_a$ denote the linear space of functions $f : G_a \to \mathbb{C}$, which are bounded in $G_a$ and for which

$$\lim_{x \to \pm \infty} f(x + iy) = 0$$

(uniformly in $|y| \leq a$) and

$$M_{\pm a}(f) = \int_{-\infty}^{\infty} |f(x \pm ia)| \, dx =$$

$$\lim_{b \uparrow a} \int_{-\infty}^{\infty} |f(x \pm ib)| \, dx < \infty.$$
The error is exponentially small

**Theorem**

Let $f \in H_a$ for some $a > 0$, and $f$ even. Then

$$|R_d(h)| \leq \frac{e^{-\pi a/h}}{\sinh(\pi a/h)} M_a(f),$$

for any $y$ with $0 < y < a$.

**Proof**

The proof is based on residue calculus.

Example: modified Bessel function

Consider the modified Bessel function

$$K_0(x) = \frac{1}{2} \int_{-\infty}^{\infty} e^{-x \cosh t} \, dt.$$

We have, with $d = 0$,

$$e^x K_0(x) = \frac{1}{2} h + h \sum_{j=1}^{\infty} e^{-x (\cosh(hj)-1)} + R_0(h).$$
For $x = 5$ and several values of $h$ we obtain ($j_0$ denotes the number of terms used in the series)

\[
\begin{array}{|c|c|c|}
\hline
h & j_0 & R_0(h) \\
\hline
1 & 2 & -1.8 \times 10^{-1} \\
1/2 & 5 & -2.4 \times 10^{-6} \\
1/4 & 12 & -6.5 \times 10^{-15} \\
1/8 & 29 & -4.4 \times 10^{-32} \\
1/16 & 67 & -1.9 \times 10^{-66} \\
1/32 & 156 & -5.5 \times 10^{-136} \\
1/64 & 355 & -1.7 \times 10^{-272} \\
\hline
\end{array}
\]
Fast convergent; easy to program

- We see in this example that, halving the value of $h$ gives a doubling of the number of significant digits.

- Roughly speaking, a doubling of the number of terms needed in the series.

- When programming this method, observe that when halving $h$, previous function values can be used.

- Details on error bounds for the remainder in this example follow from Luke (1969).
Concluding remarks

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- Sometimes the approaches in M&M are too general; the user should be alert when using these packages.

- For large variables and complex variables, quadrature methods for contour integrals are useful tools; ideas from asymptotic analysis are very fruitful here.
Thanks to Frédéric Goualard, who developed prosper
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A new \LaTeX{} class to produce high quality slides

See also SIAM News, December 2001 and

http://prosper.sourceforge.net