Arbitrary Accurate Computation with R: The Rmpfr Package

Martin Mächler
ETH Zurich

Abstract

The R package **Rmpfr** allows to use arbitrary high precision numbers instead of R's double precision numbers in many R computations and functions.

This is achieved by defining S4 classes of such numbers and vectors, matrices, and arrays thereof, where all arithmetic and mathematical functions work via the (GNU) MPFR C library, where MPFR is acronym for "***M**ultiple **P**recision **F**loating-Point **R**eliably*". MPFR is Free Software, available under the LGPL license, and itself is built on the free GNU Multiple Precision arithmetic library (GMP).

Consequently, by using **Rmpfr**, you can often call your R function or numerical code with mpfr–numbers instead of simple numbers, and all results will automatically be much more accurate.

Applications by the package author include testing of Bessel or polylog functions and distribution computations, e.g. for stable distributions.

In addition, the **Rmpfr** has been used on the `R-help` or `R-devel` mailing list for high-accuracy computations, e.g., in comparison with results from other software, and also in improving existing R functionality, e.g., fixing R bug PR#14491.

Keywords: MPFR, Abitrary Precision, Multiple Precision Floating-Point, R.

1. Introduction

There are situations, notably in researching better numerical algorithms for non-trivial mathematical functions, say the F-distribution function, where it is interesting and very useful to be able to rerun computations in R in (potentially much) higher precision.

For example, if you are interested in Euler's e, the base of natural logarithms, and given, e.g., by $e^x = \exp(x)$, you will look into

```
R> exp(1)

[1] 2.718282
```

which typically uses 7 digits for printing, as `getOption("digits")` is 7. To see R's internal accuracy fully, you can use

```
R> print(exp(1), digits = 17)

[1] 2.7182818284590451
```

With **Rmpfr** you can now simply use "mpfr – numbers" and get more accurate results automatically, here using a *vector* of numbers as is customary in R:

```
R> require("Rmpfr") # after having installed the package ...
R> (one <- mpfr(1, 120))
```

```
1 'mpfr' number of precision  120   bits
[1] 1
```

```
R> exp(one)
```

```
1 'mpfr' number of precision  120   bits
[1] 2.71828182845904523536028747135266249 79
```

In combinatorics, number theory or when computing series, you may occasionaly want to work with *exact* factorials or binomial coefficients, where e.g. you may need all factorials $k!$, for $k = 1, 2, \ldots, 24$ or a full row of Pascal's triangle, i.e., want all $\binom{n}{k}$ for $n = 80$.

With R's double precision, and standard printing precision

```
R> ns <- 1:24 ; factorial(ns)
```

```
 [1] 1.000000e+00 2.000000e+00 6.000000e+00 2.400000e+01 1.200000e+02
 [6] 7.200000e+02 5.040000e+03 4.032000e+04 3.628800e+05 3.628800e+06
[11] 3.991680e+07 4.790016e+08 6.227021e+09 8.717829e+10 1.307674e+12
[16] 2.092279e+13 3.556874e+14 6.402374e+15 1.216451e+17 2.432902e+18
[21] 5.109094e+19 1.124001e+21 2.585202e+22 6.204484e+23
```

the full precision of 24! is clearly not printed. However, if you display it with more than its full internal precision,

```
R> noquote(sprintf("%-30.0f", factorial(24)))
```

```
[1] 620448401733239409999872
```

it is obviously wrong in the last couple of digits as they are known to be 0. However, you can easily get full precision results with **Rmpfr**, by replacing "simple" numbers by mpfr-numbers:

```
R> ns <- mpfr(1:24, 120) ; factorial(ns)
```

```
24 'mpfr' numbers of precision  120   bits
 [1] 1                          2
 [3] 6                          24
 [5] 120                        720
 [7] 5040                       40320
 [9] 362880                     3628800
[11] 39916800                   479001600
[13] 6227020800                 87178291200
[15] 1307674368000              20922789888000
[17] 355687428096000            6402373705728000
[19] 121645100408832000         2432902008176640000
[21] 5109094217170944000        112400072777607680000
[23] 25852016738884976640000    620448401733239439360000
```

Or for the 80-th Pascal triangle row, $\binom{n}{k}$ for $n = 80$ and $k = 0, \ldots, n$,

```
R> chooseMpfr.all(n = 80)
```

```
80 'mpfr' numbers of precision  77 .. 128  bits
 [1] 80                         3160
 [3] 82160                      1581580
 [5] 24040016                   300500200
 [7] 3176716400                 28987537150
 [9] 231900297200               1646492110120
[11] 10477677064400             60246643120300
[13] 315136287090800            1508152231077400
[15] 6635869816740560           26958221130508525
[17] 101489773667796800         355214207837288800
[19] 1159120046626942400        3535316142212174320
```

```
[21] 10100903263463355200      270887860247426344 00
[23] 68310851714568382400      162238272822099908200
[25] 363413731121503794368     768759815833950334240
[27] 1537519631667900668480    2910305017085669122480
[29] 5218477961670854978240    8871412534840453463008
[31] 14308729894903957198400   2191024265157168446005 0
[33] 3186944385683154103280 0  4405481944914948319240 0
[35] 5790061984745360648144 0  7237577480931700810180 0
[37] 8606848896243103666160 0  9739329014169827832760 0
[39] 1048850816910596843528 00 1075072087333361764616 20
[41] 1048850816910596843528 00 9739329014169827832760 0
[43] 8606848896243103666160 0  7237577480931700810180 0
[45] 5790061984745360648144 0  4405481944914948319240 0
[47] 3186944385683154103280 0  2191024265157168446005 0
[49] 1430872989490395719840 0  8871412534840453463008
[51] 5218477961670854978240    2910305017085669122480
[53] 1537519631667900668480    7687598158339502342 40
[55] 363413731121503794368     162238272822099908200
[57] 68310851714568382400      270887860247426344 00
[59] 10100903263463355200      3535316142212174320
[61] 1159120046626942400       355214207837288800
[63] 101489773667796800        26958221130508525
[65] 6635869816740560          1508152231077400
[67] 315136287090800           60246643120300
[69] 10477677064400            1646492110120
[71] 231900297200              28987537150
[73] 3176716400                300500200
[75] 24040016                  1581580
[77] 82160                     3160
[79] 80                        1
```

S4 classes and methods: S4 allows "multiple dispatch" which means that the method that is called for a generic function may not just depend on the first argument of the function (as in S3 or in traditional class-based OOP), but on a *"signature"* of multiple arguments. For example, `a + b` is the same as `'+'(a,b)`, i.e., calling a function with two arguments.

...

1.1. The engine behind: MPFR and GMP

The package **Rmpfr** interfaces R to the C (GNU) library

> MPFR, acronym for "***M****ultiple* ***P****recision* ***F****loating-Point* ***R****eliably*".

MPFR is Free Software, available under the LGPL license, see http://mpfr.org/, and MPFR itself is built on and requires the GNU Multiple Precision arithmetic library (GMP), see http://gmplib.org/. It can be obtained from there, or from your operating system vendor.

On some platforms, it is very simple, to install MPFR and GMP, something necessary before **Rmpfr** can be used. E.g., in Linux distributions Debian, Ubuntu and other Debian derivatives, it is sufficient (for *both* libraries) to simply issue

```
sudo apt-get install libmpfr-dev
```

The standard reference to MPFR is **?**.

2. Arithmetic with mpfr-numbers

```
R> (0:7) / 7  #  k/7,  for  k= 0..7  printed with R's default precision

[1] 0.0000000 0.1428571 0.2857143 0.4285714 0.5714286 0.7142857 0.8571429
[8] 1.0000000

R> options(digits= 16)
R> (0:7) / 7  #  in full  double precision accuracy

[1] 0.0000000000000000 0.1428571428571428 0.2857142857142857
[4] 0.4285714285714285 0.5714285714285714 0.7142857142857143
[7] 0.8571428571428571 1.0000000000000000

R> options(digits=  7) # back to default
R> str(.Machine[c("double.digits","double.eps", "double.neg.eps")], digits=10)

List of 3
 $ double.digits : int 53
 $ double.eps    : num 2.220446049e-16
 $ double.neg.eps: num 1.110223025e-16

R> 2^-(52:53)

[1] 2.220446e-16 1.110223e-16
```

In other words, the double precision numbers R uses have a 53-bit mantissa, and the two "computer epsilons" are 2^{-52} and 2^{-53}, respectively.

Less technically, how many decimal digits can double precision numbers work with, $2^{-53} = 10^{-x} \iff x = 53 \log_{10}(2)$,

```
R> 53 * log10(2)

[1] 15.95459
```

i.e., almost 16 digits.

If we want to compute some arithmetic expression with higher precision, this can now easily be achieved, using the **Rmpfr** package, by defining "`mpfr`–numbers" and then work with these.

Starting with simple examples, a more precise version of $k/7$, $k = 0, \ldots, 7$ from above:

```
R> x <- mpfr(0:7, 80)/7 # using 80 bits precision
R> x

8 'mpfr' numbers of precision  80   bits
[1] 0                            0.14285714285714285714285708
[3] 0.28571428571428571428571417 0.42857142857142857142857125
[5] 0.57142857142857142857142834 0.71428571428571428571428583
[7] 0.85714285714285714285714251 1

R> 7*x

8 'mpfr' numbers of precision  80   bits
[1] 0 1 2 3 4 5 6 7

R> 7*x  - 0:7

8 'mpfr' numbers of precision  80   bits
[1] 0 0 0 0 0 0 0 0
```

which here is even "perfect" – but that's "luck" only, and also the case here for "simple" double precision numbers, at least on our current platform.[1]

[1] 64-bit Linux, Fedora 13 on a "AMD Phenom 925" processor

Our **Rmpfr** package also provides the mathematical constants which MPFR provides, via `Const(., ⟨prec⟩)`, currently the 4 constants

```
R> formals(Const)$name
```

```
c("pi", "gamma", "catalan", "log2")
```

are available, where `"gamma"` is for Euler's gamma, $\gamma := \lim_{n\to\infty} \sum_{k=1}^{n} \frac{1}{k} - \log(n) \approx 0.5777$, and `"catalan"` for Catalan's constant (see http://en.wikipedia.org/wiki/Catalan%27s_constant).

```
R> Const("pi")
```

```
1 'mpfr' number of precision  120   bits
[1] 3.1415926535897932384626433832795028847
```

```
R> Const("log2")
```

```
1 'mpfr' number of precision  120   bits
[1] 0.69314718055994530941723212145817656831
```

where you may note a default precision of 120 digits, a bit more than quadruple precision, but also that 1000 digits of π are available instantaneously,

```
R> system.time(Pi <- Const("pi", 1000 *log2(10)))
```

```
   user  system elapsed
  0.001   0.000   0.001
```

```
R> Pi
```

```
1 'mpfr' number of precision  3321   bits
[1] 3.14159265358979323846264338327950288419716939937510582097494459230781640628620899862803482534
```

TODO — an example of a user written function, computing something relevant ...

...

`seqMpfr()`

...

...

3. "All" mathematical functions, arbitrary precise

All the S4 "`Math`" group functions are defined, using multiple precision (MPFR) arithmetic, i.e.,

```
R> getGroupMembers("Math")
```

```
 [1] "abs"      "sign"     "sqrt"     "ceiling"  "floor"    "trunc"
 [7] "cummax"   "cummin"   "cumprod"  "cumsum"   "exp"      "expm1"
[13] "log"      "log10"    "log2"     "log1p"    "cos"      "cosh"
[19] "sin"      "sinh"     "tan"      "tanh"     "acos"     "acosh"
[25] "asin"     "asinh"    "atan"     "atanh"    "gamma"    "lgamma"
[31] "digamma"  "trigamma"
```

where currently , `digamma`, and `trigamma` are not provided by the MPFR library, and hence the methods not implemented yet.
Further, the `cum*()` methods are *not yet* implemented.

`factorial()` has a `"mpfr"` method; and in addition, `factorialMpfr()` computes $n!$ efficiently in arbitrary precision, using the MPFR-internal implementation. This is mathematically (but not numerically) the same as $\Gamma(n+1) =$`gamma(n+1)`.

4. Arbitrary precise matrices and arrays

... ...

... ...

5. Special mathematical functions

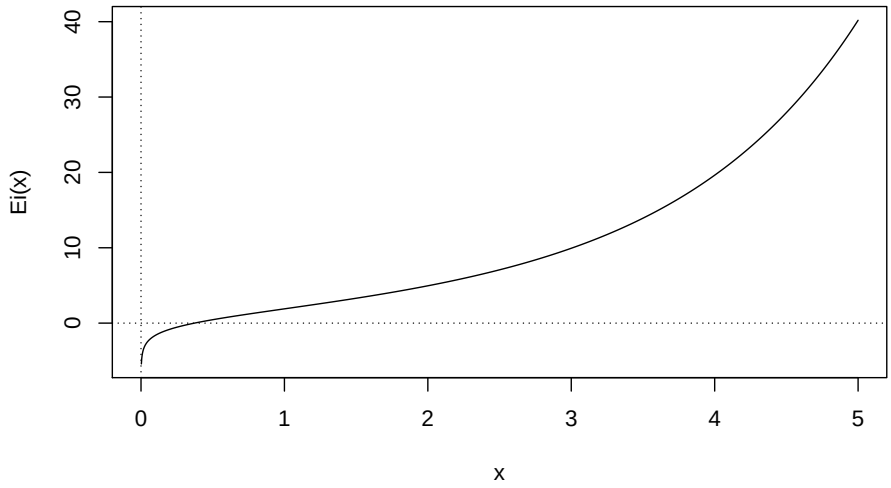
`zeta(x)` computes Riemann's Zeta function $\zeta(x)$ important in analytical number theory and related fields. The traditional definition is

$$\zeta(x) = \sum_{n=1}^{\infty} \frac{1}{n^x}.$$

`Ei(x)` computes the **e**xponential integral,

$$\int_{-\infty}^{x} \frac{e^t}{t}\, dt.$$

```
R> curve(Ei,  0, 5, n=2001);  abline(h=0,v=0, lty=3)
```



`Li2(x)`, part of the MPFR C library since version 2.4.0, computes the dilogarithm,

$$\texttt{Li2(x)} = \mathrm{Li}_2(x) := \int_0^x \frac{-log(1-t)}{t}\, dt,$$

which is the most prominent "polylogarithm" function, where the general polylogarithm is (initially) defined as

$$\mathrm{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s},\ \forall s \in \mathbb{C}\ \ \forall |z| < 1, z \in \mathbb{C},$$

see http://en.wikipedia.org/wiki/Polylogarithm#Dilogarithm.

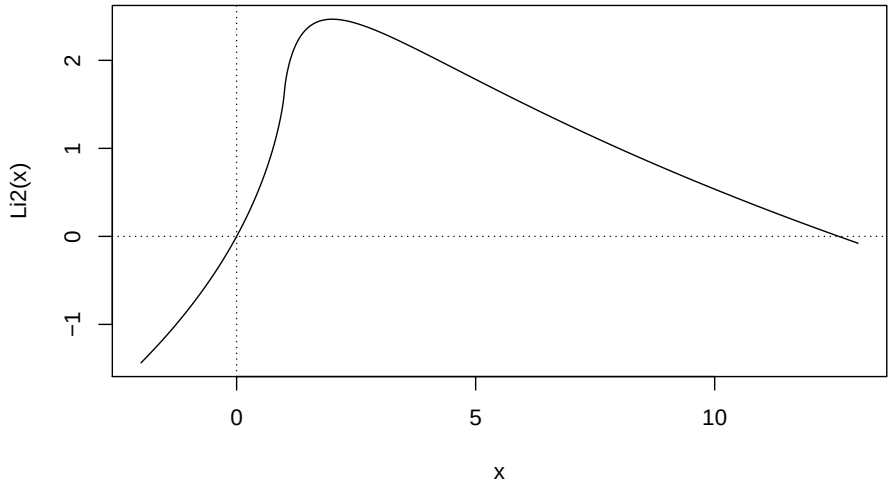
Note that the integral definition is valid for all $x \in \mathbb{C}$, and also, $Li_2(1) = \zeta(2) = \pi^2/6$.

```
R> if(mpfrVersion() >= "2.4.0")  ## Li2() is not available in older MPFR versions
   all.equal(Li2(1), Const("pi", 128)^2/6, tol = 1e-30)
```

```
[1] TRUE
```

where we also see that **Rmpfr** provides `all.equal()` methods for mpfr-numbers which naturally allow very small tolerances `tol`.

```
R> if(mpfrVersion() >= "2.4.0")
    curve(Li2, -2, 13,   n=2000); abline(h=0,v=0, lty=3)
```

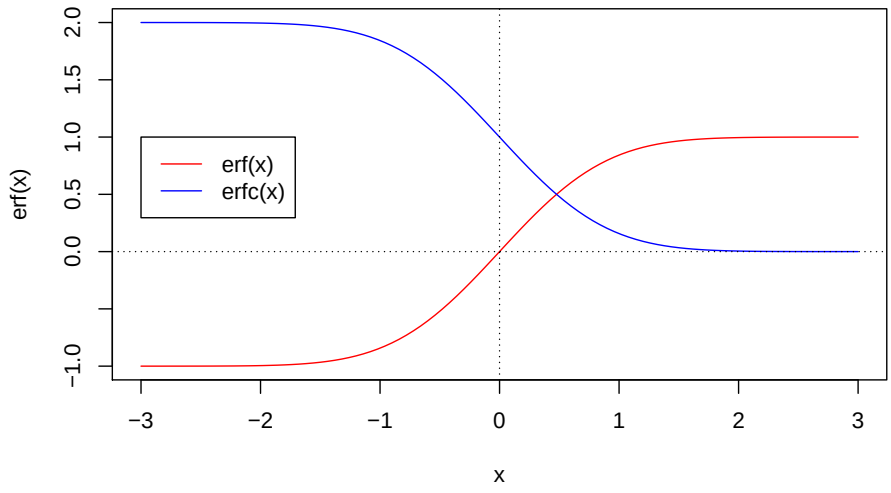


`erf(x)` is the "error[2] function" and `erfc(x)` its **c**omplement, `erfc(x) := 1 - erf(x)`, defined es

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt,$$

and consequently, both functions simply are reparametrizations of `pnorm`, `erf(x) = 2*pnorm(sqrt(2)*x)` and `erfc(x) = 1 - erf(x) = 2* pnorm(sqrt(2)*x, lower=FALSE)`.

```
R> curve(erf, -3,3, col = "red", ylim = c(-1,2))
R> curve(erfc, add = TRUE, col = "blue")
R> abline(h=0, v=0, lty=3)
R> legend(-3,1, c("erf(x)", "erfc(x)"), col = c("red","blue"), lty=1)
```



[2]named exactly because of its relation to the normal / Gaussian distribution

6. Integration highly precisely

Sometimes, important functions are defined as integrals of other known functions, e.g., the dilogarithm $\mathrm{Li}_2()$ above. Consequently, we found it desirable to allow numerical integration, using mpfr-numbers, and hence—conceptionally—arbitrarily precisely.

R's `integrate()` uses a relatively smart adaptive integration scheme, but based on C code which is not very simply translatable to pure R, to be used with mpfr numbers. For this reason, our `integrateR()` function uses classical Romberg integration (Bauer 1961).

We demonstrate its use, first by looking at a situation where R's `integrate()` can get problems:

```
R> integrateR(dnorm,0,2000)

0.5000413 with absolute error < 4.4e-05

R> integrateR(dnorm,0,2000, rel.tol=1e-15)

0.5 with absolute error < 0

R> integrateR(dnorm,0,2000, rel.tol=1e-15, verbose=TRUE)

n= 1, 2^n=        2 | I = 132.980760133811, abs.err =      265.962
n= 2, 2^n=        4 | I = 62.0576880624451, abs.err =      70.9231
n= 3, 2^n=        8 | I = 30.5363226973936, abs.err =      31.5214
n= 4, 2^n=       16 | I = 15.2082862061529, abs.err =       15.328
n= 5, 2^n=       32 | I = 7.59670992311254, abs.err =      7.61158
n= 6, 2^n=       64 | I =  3.7974274023471, abs.err =      3.79928
n= 7, 2^n=      128 | I = 1.89859780581243, abs.err =      1.89883
n= 8, 2^n=      256 | I = 0.949284417533723, abs.err =     0.949313
n= 9, 2^n=      512 | I = 0.475740259596055, abs.err =     0.473544
n=10, 2^n=     1024 | I = 0.405523469574938, abs.err =    0.0702168
n=11, 2^n=     2048 | I = 0.505758416351101, abs.err =     0.100235
n=12, 2^n=     4096 | I = 0.500041348685502, abs.err =   0.00571707
n=13, 2^n=     8192 | I = 0.499997661305352, abs.err =  4.36874e-05
n=14, 2^n=    16384 | I = 0.500000010819054, abs.err =  2.34951e-06
n=15, 2^n=    32768 | I = 0.499999999989023, abs.err =    1.083e-08
n=16, 2^n=    65536 | I = 0.500000000000003, abs.err =  1.09797e-11
n=17, 2^n=   131072 | I =               0.5, abs.err =  2.77556e-15
n=18, 2^n=   262144 | I =               0.5, abs.err =            0
0.5 with absolute error < 0
```

Now, for situtations where numerical integration would not be necessary, as the solution is known analytically, but hence are useful for exploration of high accuracy numerical integration:

First, the exponential function $\exp(x) = e^x$ with its well-known $\int \exp(t)\, dt = \exp(x)$, both with standard (double precision) floats,

```
R> (Ie.d <- integrateR(exp,            0     , 1, rel.tol=1e-15, verbose=TRUE))

n= 1, 2^n=        2 | I = 1.71886115187659, abs.err =      0.14028
n= 2, 2^n=        4 | I = 1.71828268792476, abs.err =  0.000578464
n= 3, 2^n=        8 | I = 1.71828182879453, abs.err =   8.5913e-07
n= 4, 2^n=       16 | I = 1.71828182845908, abs.err =  3.35452e-10
n= 5, 2^n=       32 | I = 1.71828182845905, abs.err =  3.30846e-14
n= 6, 2^n=       64 | I = 1.71828182845905, abs.err =            0
1.718282 with absolute error < 0
```

and then the same, using 200-bit accurate mpfr-numbers:

```
R> (Ie.m <- integrateR(exp, mpfr(0,200), 1, rel.tol=1e-25, verbose=TRUE))

n= 1, 2^n=        2 | I = 1.718861151876593, abs.err =      0.14028
n= 2, 2^n=        4 | I = 1.718282687924757, abs.err =  0.000578464
n= 3, 2^n=        8 | I = 1.71828182879453, abs.err =   8.5913e-07
n= 4, 2^n=       16 | I = 1.718281828459078, abs.err =  3.35452e-10
n= 5, 2^n=       32 | I = 1.718281828459045, abs.err =  3.30865e-14
n= 6, 2^n=       64 | I = 1.718281828459045, abs.err =  8.17815e-19
n= 7, 2^n=      128 | I = 1.718281828459045, abs.err =  5.05653e-24
n= 8, 2^n=      256 | I = 1.718281828459045, abs.err =  7.81722e-30
1.718282 with absolute error < 7.8e-30

R> (I.true <- exp(mpfr(1, 200)) - 1)

1 'mpfr' number of precision  200   bits
[1] 1.7182818284590452353602874713526624977572470936999595749669679

R> ## with absolute errors
R> as.numeric(c(I.true - Ie.d$value,
              I.true - Ie.m$value))

[1] -7.747992e-17 -7.817219e-30
```

Now, for polynomials, where romberg integration of the appropriate order is exact, mathematically,

```
R> if(require("polynom")) {
     x <- polynomial(0:1)
     p <- (x-2)^4 - 3*(x-3)^2
     Fp <- as.function(p)
     print(pI <- integral(p)) # formally
     print(Itrue <- predict(pI, 5) - predict(pI, 0)) ## == 20
 } else {
     Fp <- function(x) (x-2)^4 - 3*(x-3)^2
     Itrue <- 20
 }

-11*x - 7*x^2 + 7*x^3 - 2*x^4 + 0.2*x^5
[1] 20

R> (Id <- integrateR(Fp, 0,      5))

20 with absolute error < 7.1e-15

R> (Im <- integrateR(Fp, 0, mpfr(5, 256),
                   rel.tol = 1e-70, verbose=TRUE))

n= 1, 2^n=        2 | I = 46.04166666666666, abs.err =      98.9583
n= 2, 2^n=        4 | I =               20, abs.err =      26.0417
n= 3, 2^n=        8 | I =               20, abs.err =  2.76357e-76
20.00000 with absolute error < 2.8e-76

R> ## and the numerical errors, are indeed of the expected size:
R> 256 * log10(2) # - expect ~ 77 digit accuracy for mpfr(*., 256)

[1] 77.06368

R> as.numeric(Itrue - c(Im$value, Id$value))

[1]  2.763574e-76 -3.552714e-15
```

7. Conclusion

References

Bauer FL (1961). "Algorithm 60: Romberg integration." *Commun. ACM*, **4**, 255. ISSN 0001-0782. doi:http://doi.acm.org/10.1145/366573.366594. URL http://doi.acm.org/10.1145/366573.366594.

Fousse L, Hanrot G, Lefèvre V, Pélissier P, Zimmermann P (2011). *MPFR: A multiple-precision binary floating-point library with correct rounding*. URL http://mpfr.org/.

Granlund T, the GMP development team (2011). *GNU MP - The GNU Multiple Precision Arithmetic Library*. URL http://gmplib.org/.

Affiliation:

Martin Mächler
Seminar für Statistik, HG G 16
ETH Zurich
8092 Zurich, Switzerland
E-mail: maechler@stat.math.ethz.ch
URL: http://stat.ethz.ch/people/maechler