

Arbitrarily Accurate Computation with R: The Rmpfr Package

Martin Mächler
ETH Zurich

Abstract

The R package **Rmpfr** allows to use arbitrarily precise 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, Arbitrary 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] 2.7182818284590452353602874713526624979
```

In combinatorics, number theory or when computing series, you may occasionally want to work with *exact* factorials or binomial coefficients, where e.g. you may need all factorials $k!$, for $k = 1, 2, \dots, 24$ 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] 51090942171709440000 1124000727777607680000
[23] 25852016738884976640000 620448401733239439360000
```

Or for the 80-th Pascal triangle row, $\binom{n}{k}$ for $n = 80$ and $k = 1, \dots, n$,

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

80 'mpfr' numbers of precision 77 bits
[1] 80 3160
[3] 82160 1581580
[5] 24040016 300500200
[7] 3176716400 28987537150
.....
```

```

.....
[23]      68310851714568382400      162238272822099908200
[25]      363413731121503794368      768759815833950334240
[27]      1537519631667900668480      2910305017085669122480
[29]      5218477961670854978240      8871412534840453463008
.....
.....
[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 “*Multiple Precision Floating-Point Reliably*”.

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 Fousse, Hanrot, Lefèvre, Pélissier, and Zimmermann (2011).

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 $k/7$, $k = 0, \dots, 7$ from above:

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

```
R> x
```

```
8 'mpfr' numbers of precision 80 bits
[1] 0 0.14285714285714285714285714285708
[3] 0.28571428571428571428571417 0.42857142857142857125
[5] 0.57142857142857142857142834 0.71428571428571428583
[7] 0.8571428571428571428571425 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

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, $\gamma := \lim_{n \rightarrow \infty} \sum_{k=1}^n \frac{1}{k} - \log(n) \approx 0.5777$, 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
```

¹64-bit Linux, Fedora 13 on a “AMD Phenom 925” processor

```
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] 3.141592653589793238462643383279502884197169399375105820974944592307816406286208998628034825342
```

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

```
...
```

```
seqMpfr()
```

```
...
```

```
...
```

3. “All” mathematical functions, arbitrarily 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, `trigamma` is not provided by the MPFR library, and hence not implemented yet.

`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 $\Gamma(n+1) = \text{gamma}(n+1)$.

Similarly to `factorialMpfr()`, but more generally useful, the functions `chooseMpfr(a,n)` and `pochMpfr(a,n)` compute (generalized!) binomial coefficients $\binom{a}{n}$ and “the” Pochhammer symbol or “rising factorial”

$$\begin{aligned} a^{(n)} &:= a(a+1)(a+2) \cdots (a+n-1) \\ &= \frac{(a+n-1)!}{(a-1)!} = \frac{\Gamma(a+n)}{\Gamma(a)}. \end{aligned}$$

Note that with this definition,

$$\binom{a}{n} \equiv \frac{a^{(n)}}{n!}.$$

The classes "mpfrMatrix" and "mpfrArray" correspond to the classical numerical R "matrix" and "array" objects, which basically are arrays or vectors of numbers with a dimension `dim`, possibly named by `dimnames`. As there, they can be constructed by `dim(.) <- ..` setting, e.g.,

```
6 'mpfr' numbers of precision 64 bits
[1] 0 0.142857142857142857141 0.285714285714285714282
[4] 0.428571428571428571436 0.571428571428571428564 0.714285714285714285691
```

or by the `mpfrArray()` constructor,

[1] 2 3 4

```
'mpfrArray' of dim(.) = (2, 3, 4) of precision 80 bits
, , 1
```

[illegible]

• • • • •

• • • • •

[illegible]

```
R> mx[ 1:3, ] + c(1,10,100)
```

[,1] [,2]

```
[1,] 1.00000000000000000000 1.57142857142857142851
[2,] 10.1428571428571428570 10.7142857142857142860
[3,] 100.285714285714285712 100.857142857142857144
```

```
'mpfrMatrix' of dim(.) = (2, 2) of precision 64 bits
```

[,1] [,2]

```
[1,] 0.285714285714285714282 0.775510204081632653086
[2,] 0.775510204081632653086 2.57142857142857142851
```

```
R> apply(7 * mx, 2, sum)
```

```
2 'mpfr' numbers of precision 64 bits
[1] 6 22
```

5. Special mathematical functions

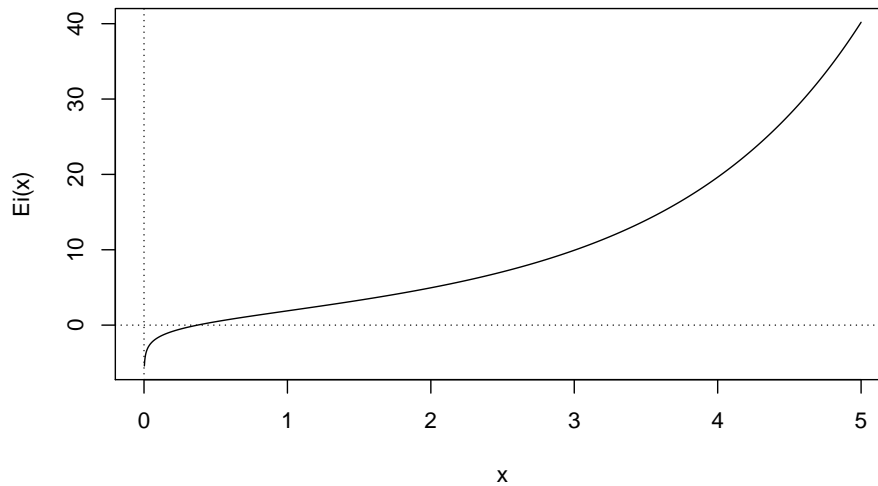
`zeta(x)` computes Riemann's Zeta function $\zeta(x)$ important in analytical number theory and related fields. The traditional definition is

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

`Ei(x)` computes the exponential 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,

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

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

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

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

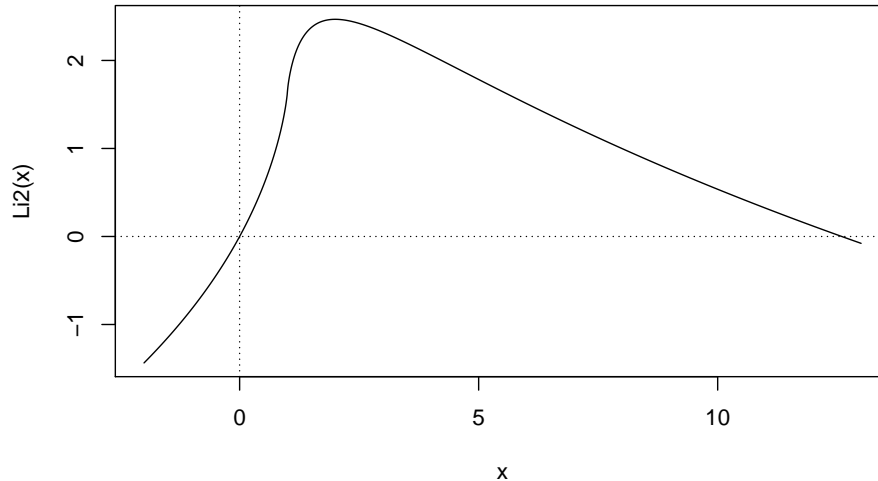
Note that the integral definition is valid for all $x \in \mathbb{C}$, and also, $\text{Li}_2(1) = \zeta(2) = \pi^2/6$.

```
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)
```

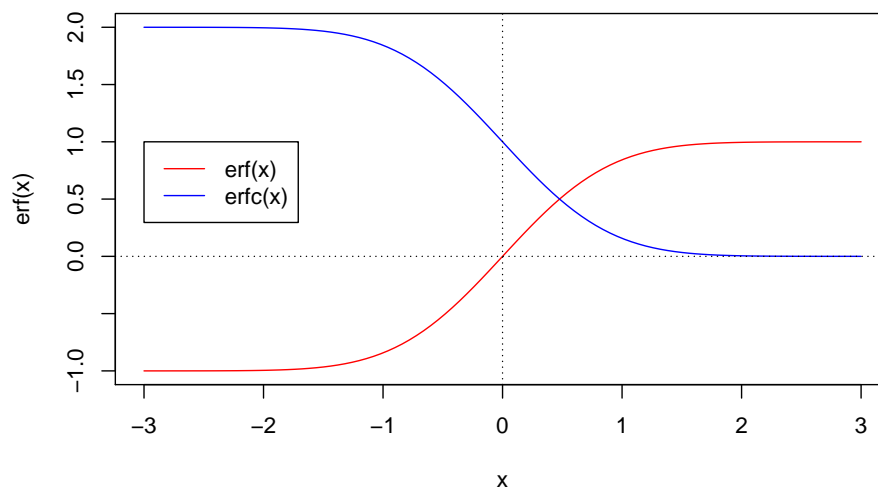


`erf(x)` is the “error² function” and `erfc(x)` its complement, `erfc(x) := 1 - erf(x)`, defined as

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

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)
```



²named 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 $\text{Li}_2()$ 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 = 132.9807601338109      , abs.err =      265.962
n= 2, 2^n=      4 | I = 62.05768806244507      , abs.err =      70.9231
n= 3, 2^n=      8 | I = 30.53632269739361      , abs.err =      31.5214
n= 4, 2^n=     16 | I = 15.20828620615289      , abs.err =       15.328
n= 5, 2^n=     32 | I = 7.596709923112541      , abs.err =       7.61158
n= 6, 2^n=     64 | I = 3.797427402347099      , abs.err =       3.79928
n= 7, 2^n=    128 | I = 1.898597805812433      , abs.err =       1.89883
n= 8, 2^n=    256 | I = 0.9492844175337234      , abs.err =       0.949313
n= 9, 2^n=    512 | I = 0.4757402595960551      , abs.err =       0.473544
n=10, 2^n=   1024 | I = 0.4055234695749382      , abs.err =      0.0702168
n=11, 2^n=   2048 | I = 0.5057584163511011      , abs.err =      0.100235
n=12, 2^n=   4096 | I = 0.5000413486855022      , abs.err =     0.00571707
n=13, 2^n=   8192 | I = 0.4999976613053521      , abs.err =    4.36874e-05
n=14, 2^n=  16384 | I = 0.5000000108190541      , abs.err =    2.34951e-06
n=15, 2^n=  32768 | I = 0.4999999999890231      , abs.err =     1.083e-08
n=16, 2^n=  65536 | I = 0.5000000000000028      , 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 situations 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 = 1.718861151876593      , 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 =    3.30846e-14
n= 6, 2^n=     64 | I = 1.718281828459045      , 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

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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>