Arbitrarily Accurate Computation with R: The Rmpfr Package

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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 (α-)stable distributions and Archimedean Copulas. 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]     51090942171709440000   1124000727777607680000
[23]  25852016738884976640000 620448401733239439360000
```

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

```
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 "***M**ultiple **P**recision **F**loating-Point **R**eliably*"

MPFR is Free Software, available under the LGPL license, see http://mpfr.org/ and Fousse, Hanrot, Lefèvre, Pélissier, and Zimmermann (2007) and the standard reference to MPFR, Fousse, Hanrot, Lefèvre, Pélissier, and Zimmermann (2011). MPFR itself is built on and requires the GNU Multiple Precision arithmetic library (GMP), see http://gmplib.org/ and Granlund and the GMP development team (2011). 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
```

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]  0.85714285714285714285714425                             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, $\gamma := \lim_{n\to\infty} \sum_{k=1}^{n} \frac{1}{k} - \log(n) \approx 0.5777$, 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
```

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

```
R> Const("log2")

1 'mpfr' number of precision  120   bits
[1] 0.693147180559945309417232121458176568 31
```

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 2
```

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"    "cospi"    "sinpi"
[31] "tanpi"    "gamma"    "lgamma"   "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 $\Gamma(n+1)$ =`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,

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

4. Arbitrarily precise matrices and arrays

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.,

```
R> head(x <- mpfr(0:7, 64)/7) ; mx <- x

6 'mpfr' numbers of precision  64   bits
[1]                        0 0.14285714285714285141 0.28571428571428571282
[4] 0.42857142857142857436 0.57142857142857142564 0.71428571428571428691

R> dim(mx) <- c(4,2)
```

or by the `mpfrArray()` constructor,

```
R> dim(aa <- mpfrArray(1:24, precBits = 80, dim = 2:4))

[1] 2 3 4

R> aa

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

     [,1]                          [,2]
[1,] 1.0000000000000000000000000 3.0000000000000000000000000
[2,] 2.0000000000000000000000000 4.0000000000000000000000000
     [,3]
[1,] 5.0000000000000000000000000
[2,] 6.0000000000000000000000000

, , 2
 .......
 .......
     [,3]
[1,] 23.000000000000000000000000
[2,] 24.000000000000000000000000
```

and we can index and multiply such matrices, e.g.,

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

'mpfrMatrix' of dim(.) =  (3, 2) of precision  64   bits
     [,1]                    [,2]
[1,] 1.00000000000000000000 1.57142857142857142851
[2,] 10.14285714285714285570 10.71428571428571428560
[3,] 100.28571428571428571282 100.85714285714285714144

R> crossprod(mx)

'mpfrMatrix' of dim(.) =  (2, 2) of precision  64   bits
     [,1]                      [,2]
[1,] 0.28571428571428571282 0.77551020408163265306
[2,] 0.77551020408163265306  2.57142857142857142851
```

and also `apply` functions,

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

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

5. Special mathematical functions

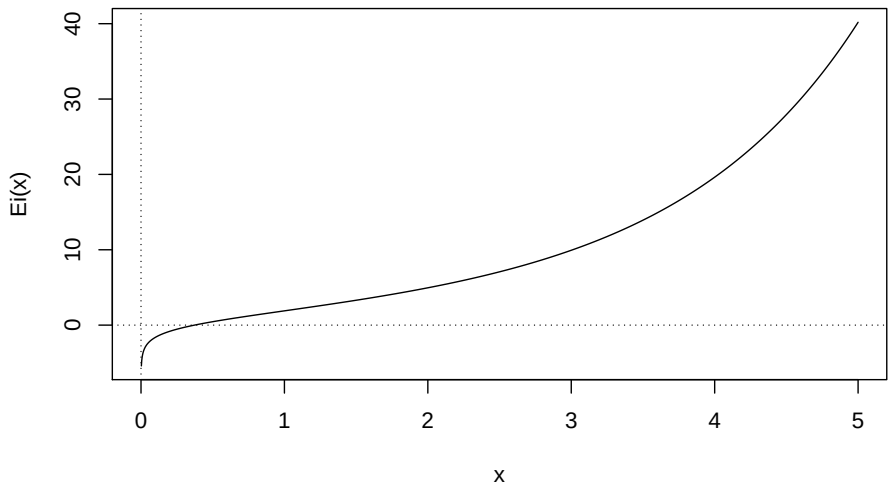
`zeta(x)` computes Riemann's Zeta function $\zeta(x)$ important in analytical number theory and related fields. The traditional definition is

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

`Ei(x)` computes the **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

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

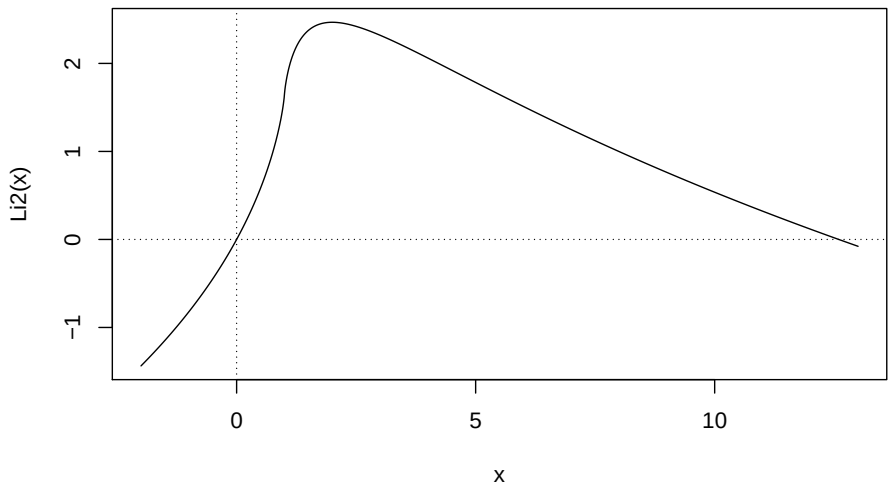
see http://en.wikipedia.org/wiki/Polylogarithm#Dilogarithm.

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)
```



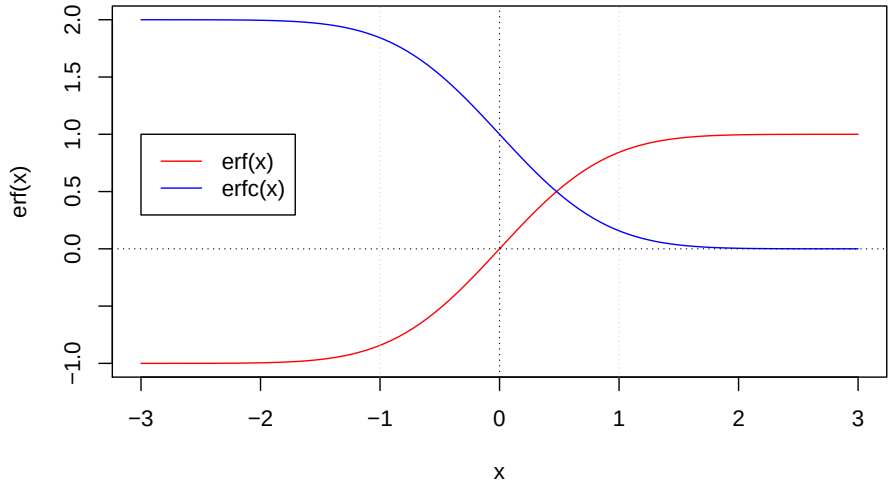
`erf(x)` is the "error[2] function" and `erfc(x)` its **c**omplement, `erfc(x) := 1 - erf(x)`, defined as

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

and consequently, both functions simply are reparametrizations of the cumulative normal, $\Phi(x) = \int_{-\infty}^{x} \phi(t)\, dt =$`pnorm(x)` where ϕ is the normal density function $\phi(t) := \frac{1}{\sqrt{2\pi}} e^{-t^2} =$`dnorm(x)`. Namely, `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); abline(v=c(-1,1), lty=3, lwd=.8, col="gray")
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



5.1. Applications

The CRAN package **Bessel**

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)

0.5 with absolute error < 4.3687e-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)

ord = 25 will be the *maximal* order
n= 1, 2^n=        2 | I =     132.98076013381089, abs.err =      265.9615
n= 2, 2^n=        4 | I =     62.057688062445074, abs.err =      70.92307
n= 3, 2^n=        8 | I =     30.536322697393608, abs.err =      31.52137
n= 4, 2^n=       16 | I =     15.208286206152895, abs.err =      15.32804
n= 5, 2^n=       32 | I =     7.5967099231125408, abs.err =      7.611576
n= 6, 2^n=       64 | I =     3.7974274023470991, abs.err =      3.799283
n= 7, 2^n=      128 | I =     1.8985978058124329, abs.err =       1.89883
n= 8, 2^n=      256 | I =    0.94928441753372339, abs.err =     0.9493134
n= 9, 2^n=      512 | I =    0.47574025959605515, abs.err =     0.4735442
```

```
n=10, 2^n=     1024 | I =    0.40552346957493818, abs.err =    0.07021679
n=11, 2^n=     2048 | I =    0.50575841635110108, abs.err =     0.1002349
n=12, 2^n=     4096 | I =    0.50004134868550221, abs.err =   0.005717068
n=13, 2^n=     8192 | I =    0.49999766130535211, abs.err =  4.368738e-05
n=14, 2^n=    16384 | I =     0.5000000108190541, abs.err =  2.349514e-06
n=15, 2^n=    32768 | I =    0.49999999998902311, abs.err =  1.083003e-08
n=16, 2^n=    65536 | I =    0.50000000000000278, abs.err =  1.097966e-11
n=17, 2^n=   131072 | I =                    0.5, abs.err =  2.775558e-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))

ord = 25 will be the *maximal* order
n= 1, 2^n=        2 | I =     1.7188611518765928, abs.err =     0.1402798
n= 2, 2^n=        4 | I =     1.7182826879247572, abs.err =   0.000578464
n= 3, 2^n=        8 | I =     1.7182818287945303, abs.err =  8.591302e-07
n= 4, 2^n=       16 | I =     1.7182818284590784, abs.err =  3.354519e-10
n= 5, 2^n=       32 | I =     1.7182818284590453, abs.err =  3.308465e-14
n= 6, 2^n=       64 | I =     1.7182818284590453, abs.err =             0
1.7183 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))

ord = 25 will be the *maximal* order
n= 1, 2^n=        2 | I =     1.7188611518765929704591484 4, abs.err =     0.1402798
n= 2, 2^n=        4 | I =     1.7182826879247574588167457 1, abs.err =  0.0005784640
n= 3, 2^n=        8 | I =     1.7182818287945304231525787 3, abs.err =   8.591302e-7
n= 4, 2^n=       16 | I =     1.7182818284590783226601035 8, abs.err =  3.354521e-10
n= 5, 2^n=       32 | I =     1.7182818284590452361781075 7, abs.err =  3.308648e-14
n= 6, 2^n=       64 | I =     1.7182818284590452353602925 3, abs.err =  8.178150e-19
n= 7, 2^n=      128 | I =     1.7182818284590452353602874 7, abs.err =  5.056528e-24
n= 8, 2^n=      256 | I =     1.7182818284590452353602874 7, abs.err =  7.817216e-30
1.7183 with absolute error < 7.8172e-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 -3.021394e-36
```

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 < 7.1054e-15

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

ord = 25 will be the *maximal* order
n= 1, 2^n=        2 | I =     46.041666666666666666666666666666666666666666666667, abs.err =      9
n= 2, 2^n=        4 | I =     20.000000000000000000000000000000000000000000000000, abs.err =      2
n= 3, 2^n=        8 | I =     20.000000000000000000000000000000000000000000000000, abs.err =  2.763
20.000 with absolute error < 2.7636e-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] 0.000000e+00 3.552714e-15
```

7. Conclusion

The R package **Rmpfr**, available from CRAN since August 2009, provides the possibility to run many computations in R with (arbitrarily) high accuracy, though typically with substantial speed penalty.

This is particularly important and useful for checking and exploring the numerical stability and appropriateness of mathematical formulae that are translated to a computer language like R, often without very careful consideration of the limits of computer arithmetic.

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