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 "*Multiple Precision Floating-Point Reliably*". 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 $(\alpha$ -)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] 2.7182818284590452353602874713526624979
```

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, ..., 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)</pre>

```
[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
 [1]
                             1
                                                        2
 [3]
                                                       24
                             6
 [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
       5218477961670854978240
                                 8871412534840453463008
[29]
[77]
                         82160
                                                    3160
[79]
                            80
```

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 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 1.00000000000000

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 \leftarrow mpfr(0:7, 80)/7 \# using 80 bits precision
R> x
8 'mpfr' numbers of precision 80
                                0 0.14285714285714285714285708
[1]
[3] 0.28571428571428571428571417 0.42857142857142857142857125
[5] 0.57142857142857142857142834 0.71428571428571428571428583
[7] 0.8571428571428571428571425
                                                              1
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

2.1. Mathematical Constants, Pi (π) , gamma, etc

Our **Rmpfr** package also provides the mathematical constants which MPFR provides, via $Const(., \langle prec \rangle)$, 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).

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

```
R> Const("pi")
1 'mpfr' number of precision 120
[1] 3.1415926535897932384626433832795028847
R> Const("log2")
1 'mpfr' number of precision 120
[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 \pi are available instantaneously,
R> system.time(Pi <- Const("pi", 1000 *log2(10)))</pre>
  user system elapsed
 0.001
        0.000
                0.002
R> Pi
1 'mpfr' number of precision 3321
                                 bits
As nice example of using Mpfr arithmetic: On a wintery Sunday, Hans Borchers desired
to have an exact \pi constant in Rmpfr, and realized that of course mpfr(pi, 256) could
```

As nice example of using Mpfr arithmetic: On a wintery Sunday, Hans Borchers desired to have an exact π constant in **Rmpfr**, and realized that of course mpfr(pi, 256) could not be the solution, as pi is the double precision version of π and hence only about 53 bit accurate (and the mpfr() cannot do magic, recognizing "symbolic" π). As he overlooked the Const("pi", .) solution above, he implemented the following function that computes pi applying Gauss' spectacular AGM-based (AGM := Arithmetic-Geometric Mean) approach [Borwein and Borwein (1987), Pi and the AGM]; I have added a verbose argument, explicit iteration counting and slightly adapted the style to my own:

```
R> piMpfr <- function(prec=256, itermax = 100, verbose=TRUE) {
       m2 <- mpfr(2, prec) # '2' as mpfr number</pre>
       ## -> all derived numbers are mpfr (with precision 'prec')
       p \leftarrow m2 + sqrt(m2) # 2 + sqrt(2) = 3.414..
       y <- sqrt(sqrt(m2)) # 2^ {1/4}
       x < - (y+1/y) / m2
       it <- 0L
       repeat {
           p.old <- p
            it <- it+1L
           p < -p * (1+x) / (1+y)
            if(verbose) cat(sprintf("it=%2d, pi^ = %s, |.-.|/|.|=%e\n",
                                     it, formatMpfr(p, min(50, prec/log2(10))), 1-p.old/p))
            if (abs(p-p.old) \le m2^(-prec))
                break
            if(it > itermax) {
                warning("not converged in", it, "iterations") ; break
            }
            ## else
            s \leftarrow sqrt(x)
            y \leftarrow (y*s + 1/s) / (1+y)
            x \leftarrow (s+1/s)/2
       }
       р
R> piMpfr()# indeed converges *quadratically* fast
```

```
it= 1, pi^ = 3.1426067539416226007907198236183018919713562462772, |.-.|/|.|=-8.642723e-02
it= 2, pi^ = 3.1415926609660442304977522351203396906792842568645, |.-.|/|.|=-3.227958e-04
it= 3, pi^ = 3.1415926535897932386457739917571417940347896238675, |.-.|/|.|=-2.347934e-09
it= 4, pi^ = 3.1415926535897932384626433832795028841972241204666, |.-.|/|.|=-5.829228e-20
it= 5, pi^ = 3.1415926535897932384626433832795028841971693993751, |.-.|/|.|=-1.741826e-41
it= 6, pi^ = 3.1415926535897932384626433832795028841971693993751, |.-.|/|.|=0.000000e+00
1 'mpfr' number of precision 256 bits
[1] 3.141592653589793238462643383279502884197169399375105820974944592307816406286163
R> ## with relative error
R> relErr <- 1 - piMpfr(256, verbose=FALSE) / Const("pi",260)
R> ## in bits :
R> asNumeric(-log2(abs(relErr)))
[1] 255.2451
```

2.2. seqMpfr() for sequences:

0.30103....

In R, arithmetic sequences are constructed by seq(), the "sequence" function, which is not generic, and with its many ways and possible arguments is convenient, but straightforward to automatically generalize for mpfr numbers. Instead, we provide the seqMpfr function...

2.3. Rounding, roundMpfr(), asNumeric() etc:

In R, the round() and signif() functions belong to the Math2 group, and we provide "mpfr"-class methods for them:

```
R> getGroupMembers("Math2")
[1] "round" "signif"
R> showMethods("Math2", classes=c("mpfr", "mpfrArray"))
Function: Math2 (package methods)
x="mpfr"
For consistency reasons, however the resulting numbers keep the same number of precision
bits, precBits:
R > i7 < -1/mpfr(700, 100)
R > c(i7, round(i7, digits = 6), signif(i7, digits = 6))
3 'mpfr' numbers of precision 100
[1] 0.001428571428571428571428571428571
[3] 0.0014285699999999999999999999999999999
If you really want to "truncate" the precision to less digits or bits, you call roundMpfr(),
R> roundMpfr(i7, precBits = 30)
1 'mpfr' number of precision 30
                                   bits
[1] 0.0014285714278
R> roundMpfr(i7, precBits = 15)
1 'mpfr' number of precision 15
[1] 0.00142854
Note that 15 bits correspond to approximately 15 \cdot 0.3, i.e., 4.5 digits, because 1/\log_2(10) \approx
```

asNumeric(): Often used, e.g., to return to fast (R-internal) arithmetic, also as alternative to roundMpfr() is to "round to double precision" producing standard Rnumbers from "mpfr" numbers. We provide the function asNumeric(), a generic function with methods also for "mpfrArray" see below and the big integers and big rationals from package gmp,

R> showMethods(asNumeric)

Formatting: For explicit printing or plotting purposes, we provide an "mpfr" method for R's format() function, also as explicit utility function formatMpfr(x, digits) which provides results to digits significant digits,

```
R> cbind( sapply(1:7, function(d) format(i7, digits=d)) )
```

```
[,1]
[1,] "0.001"
[2,] "0.0014"
[3,] "0.00143"
[4,] "0.001429"
[5,] "0.0014286"
[6,] "0.00142857"
[7,] "0.001428571"
```

There, digits = NULL is the default where the help has ("always") promised The default, NULL, uses enough digits to represent the full precision, often one or two digits more than you would expect. However, for large numbers, say 10^{20000} , e.g., new("mpfr1", prec = 80, exp = c(66439,0), sign = 1, d = c(0,-1008336896,1315775171,-1124830946)), all of formatMpfr(x), format(x), and print(x) (including "auto-printing" of x), have shown all digits before the decimal point and not at all taken into account the 80-bit precision of x (which corresponds to only 80 / log2(10) \approx 24 decimal digits). This has finally changed in the (typically default) case formatMpfr(*, maybe.full = FALSE):

[1] 3012 6022 9033 12043

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

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"

$$a^{(n)} := a(a+1)(a+2)\cdots(a+n-1)$$

= $\frac{(a+n-1)!}{(a-1)!} = \frac{\Gamma(a+n)}{\Gamma(a)}$.

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 \leftarrow mpfr(0:7, 64)/7); mx <- x 
6 'mpfr' numbers of precision 64 bits 
[1] 0 0.142857142857142857141 0.285714285714285714282 
[4] 0.428571428571428571436 0.571428571428564 0.714285714285714285691 
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
'mpfrArray' of dim(.) = (2, 3, 4) of precision 80
                                       bits
, , 1
   [,1]
                        [,2]
, , 2
. . . . . . .
   [,3]
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,] 1.0000000000000000000 1.57142857142857142851
[2,] 10.1428571428571428570 10.7142857142857142860
[3,] 100.285714285714285712 100.857142857142857144
R> crossprod(mx)
'mpfrMatrix' of dim(.) = (2, 2) of precision 64
[1,] 0.285714285714285714282 0.775510204081632653086
[2,] 0.775510204081632653086 2.57142857142857142851
and also apply functions,
R > apply(7 * mx, 2, sum)
2 'mpfr' numbers of precision 64
[1] 6 22
```

5. Special mathematical functions

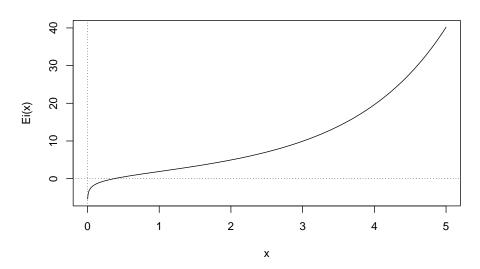
zeta(x) computes Riemann's Zeta function $\zeta(x)$ important in analytical number theory and related fields. The traditional definition is

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

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,

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

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

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

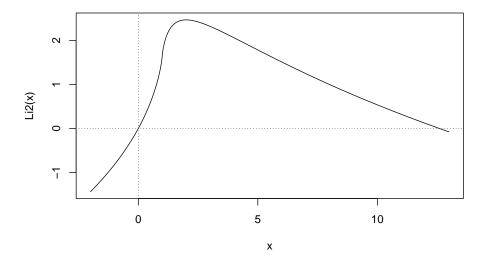
see http://en.wikipedia.org/wiki/Polylogarithm#Dilogarithm.

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.

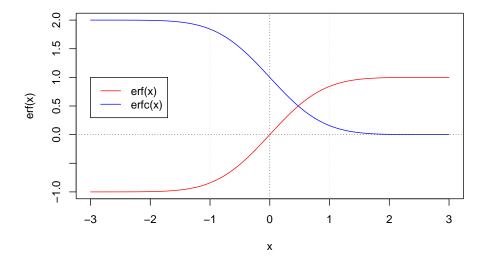


erf(x) is the "error² function" and erfc(x) its complement, erfc(x) := 1 - erf(x), defined as

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

and consequently, both functions simply are reparametrizations of the cumulative normal, $\Phi(x) = \int_{-\infty}^x \phi(t) \ dt = \texttt{pnorm}(\texttt{x}) \text{ where } \phi \text{ is the normal density function } \phi(t) := \frac{1}{\sqrt{2\pi}} e^{-t^2} = \texttt{dnorm}(\texttt{x}).$ 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

0.07021679

0.1002349

0.005717068

4.368738e-05

2.349514e-06

1.083003e-08

1.097966e-11

5.1. Applications

 $n=10, 2^n=$

n=11, 2^n=

n=12, 2ⁿ⁼

n=13, 2ⁿ=

 $n=14, 2^n=$

n=15, 2ⁿ⁼

n=16, 2ⁿ=

n=17, 2ⁿ=

n=18, 2ⁿ=

1024 | I =

2048 | I =

4096 | I =

8192 | I =

16384 | I =

32768 | I =

65536 | I =

131072 | I =

262144 | I =

0.5 with absolute error < 0

The CRAN package **Bessel** provides asymptotic formulas for Bessel functions also of *fractional* order which do work for mpfr-vector arguments as well.

6. Integration highly precisely

Sometimes, important functions are defined as integrals of other known functions, e.g., the dilogarithm Li₂() 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)
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
                 16 | I =
n=4, 2^n=
                               15.208286206152895, abs.err =
                                                                    15.32804
n= 5, 2<sup>n</sup>=
                 32 | I =
                               7.5967099231125408, abs.err =
                                                                    7.611576
                 64 | I =
n=6, 2^n=
                               3.7974274023470991, abs.err =
                                                                    3.799283
                               1.8985978058124329, abs.err =
                 128 | I =
n= 7, 2^n=
                                                                     1.89883
n= 8, 2<sup>n</sup>=
                256 | I =
                              0.94928441753372339, abs.err =
                                                                   0.9493134
n= 9, 2^n=
                512 | I =
                              0.47574025959605515, abs.err =
                                                                   0.4735442
```

```
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:
```

0.40552346957493818, abs.err =

0.50575841635110108, abs.err =

0.50004134868550221, abs.err =

0.49999766130535211, abs.err =

0.5000000108190541, abs.err =

0.499999999999311, abs.err =

0.50000000000000278, abs.err =

0.5, abs.err =

0.5, abs.err =

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))
```

```
1.7188611518765928, abs.err = 0.1402798
1.7182826879247572, abs.err = 0.000578464
1.7182818287945303, abs.err = 8.591302e-07
n=1, 2^n=
                   2 | I =
n= 2, 2^n=
                   4 | I =
                   8 | I =
n= 3, 2<sup>n=</sup>
                   16 | I =
n=4, 2^n=
                              1.7182818284590784, abs.err = 3.354519e-10
                   32 | I = 1.7182818284590453, abs.err = 3.308465e-14
64 | I = 1.7182818284590453, abs.err = 0
n= 5, 2<sup>n=</sup>
n= 6, 2^n=
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))
n=1, 2^n=
                   2 | I = 1.71886115187659297045914844, abs.err =
                   1.7182818286792475745881674571, abs.err = 0.0005784640

8 | I = 1.71828182879453042315257873, abs.err = 8.591302e-7

16 | I = 1.71828182845907832266010358, abs.err = 3.354521e-10

32 | I = 1.71828182845904523617810757, abs.err = 3.308648e-14
n= 2, 2^n=
n= 3, 2^n=
                   16 | I =
n=4, 2^n=
                  32 | I =
n= 5, 2<sup>n=</sup>
                  64 | I = 1.71828182845904523536029253, abs.err = 8.178150e-19
n= 6, 2<sup>n=</sup>
               128 | I = 1.71828182845904523536028747, abs.err = 5.056528e-24
256 | I = 1.71828182845904523536028747, abs.err = 7.817216e-30
n= 7, 2^n=
n= 8, 2^n=
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, mathe-
matically,
R> if(require("polynom")) {
        x \leftarrow polynomial(0:1)
        p \leftarrow (x-2)^4 - 3*(x-3)^2
       Fp <- as.function(p)</pre>
       print(pI <- integral(p)) # formally</pre>
       print(Itrue <- predict(pI, 5) - predict(pI, 0)) ## == 20</pre>
   } else {
       Fp \leftarrow 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,</pre>
20 with absolute error < 7.1054e-15
R> (Im <- integrateR(Fp, 0, mpfr(5, 256),</pre>
                       rel.tol = 1e-70, verbose=TRUE))
n= 1, 2^n=
                                 n= 2, 2<sup>n</sup>=
                    4 | I =
                                 8 | I =
n= 3, 2^n=
                                 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. Miscellaneous

For probability and density computations, it is known to be important in many contexts to work on the log-scale, i.e., with log probabilities $\log P(.)$ or log densities $\log f()$. In R itself, we (R Core) had introduced logical optional arguments \log (for density) and \log p for probability (e.g., pnorm() and quantile (e.g., qnorm) functions.

As our pnorm() is based on MPFR's erf() and erfc() which currently do *not* have scaled versions, for Rmpfr::pnorm(.., log.p=TRUE) we do need to compute the logarithm (instead of working on the log scale). On the extreme left tail, R correctly computes

```
R> pnorm(-1234, log.p=TRUE)
```

```
[1] -761386
```

i.e., -761386.036955 to more digits. However, erf() and erfc() do not have a log scale or other scaled versions.

Thanks to the large range of exponents compared to double precision numbers it does less quickly underflow to zero, e.g.,

```
R > (p123 \leftarrow Rmpfr::pnorm(mpfr(-123, 66), log.p=TRUE)) # is based on
1 'mpfr' number of precision 66
                                    bits
[1] -7570.23118897588017062
R> (ec123 <- erfc(123 * sqrt(mpfr(0.5, 66+4))) / 2) # 1.95....e-3288
1 'mpfr' number of precision 70
[1] 1.9514970354854432606612e-3288
R> (p333 <- Rmpfr::pnorm(mpfr(-333, 66), log.p=TRUE))
1 'mpfr' number of precision 66
                                    bits
[1] -55451.2270900410088492
R > \exp(p333)
1 'mpfr' number of precision 66
[1] 6.88747493033304647776e-24083
R> stopifnot(p123 == log(roundMpfr(ec123, 66)), ## '==' as we implemented our pnorm()
             all.equal(p333, -55451.22709, tol=1e-8))
and indeed, the default range for exponent (wrt base 2, not 10) is given by
R> (old_erng <- .mpfr_erange() )</pre>
       Emin
                   Emax
-1073741823 1073741823
```

which shows the current minimal and maximal base-2 exponents for mpfr-numbers, by "factory-fresh" default, the number -2^{30} and 2^{30} , i.e., ± 1073741823 which is much larger than the corresponding limits for regular double precision numbers,

which are basically $\pm 2^{10}$; note that double arithmetic typically allows subnormal numbers which are even smaller than 2^{-1024} , also in R, on all usual platforms,

```
R> 2^(-1022 - 52)
```

[1] 4.940656e-324

is equal to 2^{-1074} and the really smallest positive double precision number.

Now, if if the GMP library to which both R package **gmp** and **Rmpfr** interface is built "properly", i.e., with full 64 bit "numb"s, we can extend the range of mpfr-numbers even further. By how much, we can read off

```
R> .mpfr_erange(.mpfr_erange_kinds) ## and then set
```

```
min.emin
                                                max.emin
-1.073742e+09
               1.073742e+09 -4.611686e+18 4.611686e+18 -4.611686e+18
     max.emax
 4.611686e+18
R> # use very slightly smaller than extreme values:
R> (myERng <- (1-2^-52) * .mpfr_erange(c("min.emin", "max.emax")))
     min.emin
                   max.emax
-4.611686e+18 4.611686e+18
R> .mpfr_erange_set(value = myERng) # and to see what happened:
R> .mpfr_erange()
         F.min
                       Emax
-4.611686e+18 4.611686e+18
```

If that worked well, this shows -/+ 4.611686e+18, or actually $\mp 2^{62}$, log2(abs(.mpfr_erange())) giving 62.

However, currently on Winbuilder this does not extend, notably as the GMP numbs,

```
R> .mpfr_gmp_numbbits()
```

[1] 64

have not been 64, there.

8. 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.

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 (2007). "MPFR: A multiple-precision binary floating-point library with correct rounding." *ACM Trans. Math. Softw.*, **33**(2), 13. ISSN 0098-3500. URL http://doi.acm.org/10.1145/1236463.1236468.

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/.

FIXME: **Index** of all functions mentioned ...

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