expint: Exponential integral and incomplete gamma function

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1 Introduction

The exponential integral

$$E_1(x) = \int_x^\infty \frac{e^{-t}}{t}\,dt, \quad x \in \mathbb{R}$$

and the incomplete gamma function

$$\Gamma(a, x) = \int_x^\infty t^{a-1}e^{-t}\,dt, \quad x > 0, \quad a \in \mathbb{R}$$

are two closely related functions that arise in various fields of mathematics.

expint is a small package that intends to fill a gap in R's support for mathematical functions by providing facilities to compute the exponential integral and the incomplete gamma function. Furthermore, and perhaps most conveniently for R package developers, the package also gives easy access to the underlying C workhorses through an API. The C routines are derived from the GNU Scientific Library (GSL; Galassi et al., 2009).

Package **expint** started its life in version 2.0-0 of package **actuar** (Dutang et al., 2008) where we extended the range of admissible values in the computation of limited expected value functions. This required an incomplete gamma function that accepts negative values of argument a, as explained at the beginning of Appendix A of Klugman et al. (2012).

2 Exponential integral

Abramowitz and Stegun (1972, Section 5.1) first define the exponential integral as

$$E_1(x) = \int_x^\infty \frac{e^{-t}}{t}\,dt. \tag{1}$$

An alternative definition (to be understood in terms of the Cauchy principal value due to the singularity of the integrand at zero) is

$$\mathrm{Ei}(x) = -\int_{-x}^{\infty} \frac{e^{-t}}{t}\, dt = \int_{-\infty}^{x} \frac{e^{t}}{t}\, dt, \quad x > 0.$$

The above two definitions are related as follows:

$$E_1(-x) = -\mathrm{Ei}(x), \quad x > 0. \tag{2}$$

The exponential integral can also generalized to

$$E_n(x) = \int_1^{\infty} \frac{e^{-xt}}{t^n}\, dt, \quad n = 0, 1, 2, \ldots, \quad x > 0,$$

where n is then the *order* of the integral. The latter expression is closely related to the incomplete gamma function (section 3) as follows:

$$E_n(x) = x^{n-1}\Gamma(1-n, x). \tag{3}$$

One should note that the first argument of function Γ is negative for $n > 1$.

The following recurrence relation holds between exponential integrals of successive orders:

$$E_{n+1}(x) = \frac{1}{n}[e^{-x} - xE_n(x)]. \tag{4}$$

Finally, $E_n(x)$ has the following asymptotic expansion:

$$E_n(x) \asymp \frac{e^{-x}}{x}\left(1 - \frac{n}{x} + \frac{n(n+1)}{x^2} - \frac{n(n+1)(n+2)}{x^3} + \ldots\right). \tag{5}$$

3 Incomplete gamma function

From a probability theory perspective, the incomplete gamma function is usually defined as

$$P(a, x) = \frac{1}{\Gamma(a)} \int_0^x t^{a-1} e^{-t}\, dt, \quad x > 0, \quad a > 0.$$

Function `pgamma` already implements this function in R (just note the differing order of the arguments).

Now, the definition of the incomplete gamma function of interest for this package is rather the following (Abramowitz and Stegun, 1972, Section 6.5):

$$\Gamma(a, x) = \int_x^{\infty} t^{a-1} e^{-t}\, dt, \quad x > 0, \quad a \in \mathbb{R}. \tag{6}$$

Note that a can be negative with this definition. Of course, for $a > 0$ one has

$$\Gamma(a, x) = \Gamma(a)[1 - P(a, x)]. \tag{7}$$

Integration by parts of the integral in (6) yields the relation

$$\Gamma(a,x) = -\frac{x^a e^{-x}}{a} + \frac{1}{a}\Gamma(a+1,x).$$

When $a < 0$, this relation can be used repeatedly k times until $a+k$ is a positive number. The right hand side can then be evaluated with (7). If $a = 0, -1, -2, \ldots$, this calculation requires the value of

$$G(0,x) = \int_x^\infty \frac{e^{-t}}{t}\, dt = E_1(x),$$

the exponential integral defined in (1).

4 R interfaces

Package **expint** provides one main and four auxiliary R functions to compute the exponential integral, and one function to compute the incomplete gamma function. The synopses of these are the following:

```
expint(x, order = 1L, scale = FALSE)
expint_E1(x, scale = FALSE)
expint_E2(x, scale = FALSE)
expint_En(x, order, scale = FALSE)
expint_Ei(x, scale = FALSE)
gammainc(a, x)
```

Let us first go over function `gammainc` since there is less to discuss. The function takes in argument two vectors or real numbers (non-negative for argument `x`) and returns the value of $\Gamma(a,x)$. The function is vectorized in arguments `a` and `x`, so it works similar to, say, `pgamma`.

We now turn to the `expint` family of functions. Function `expint` is a unified interface to compute exponential integrals $E_n(x)$ of any (non-negative) order, with default the most common case $E_1(x)$. The function is vectorized in arguments `x` and `order`. In other words, one can compute the exponential integral of a different order for each value of x.

```
> expint(c(1.275, 10, 12.3), order = 1:3)
[1] 1.408099e-01 3.830240e-06 3.009983e-07
```

Argument `order` should be a vector of integers. Non-integer values are silently coerced to integers using truncation towards zero.

When argument `scale` is `TRUE`, the result is scaled by e^x.

Functions `expint_E1`, `expint_E2` and `expint_En` are simpler, slightly faster ways to directly compute exponential integrals $E_1(x)$, $E_2(x)$ and $E_n(x)$, the latter for a *single* order n (the first value of `order` if `order` is a vector).

```
> expint_E1(1.275)
[1] 0.1408099
> expint_E2(10)
[1] 3.83024e-06
> expint_En(12.3, order = 3L)
[1] 3.009983e-07
```

Finally, function `expint_Ei` is provided as a convenience to compute $\mathrm{Ei}(x)$ using (2).

```
> expint_Ei(5)
[1] 40.18528
> -expint_E1(-5)     # same
[1] 40.18528
```

5 Accessing the C routines

The actual workhorses behind the R functions of section 4 are C routines with the following prototypes:

```
double expint_E1(double x, int scale);
double expint_E2(double x, int scale);
double expint_En(double x, int order, int scale);
double gamma_inc(double a, double x);
```

Package **expint** makes these routines available to other packages through declarations in the header file 'include/expintAPI.h' in the package installation directory. The developer of some package **pkg** who wants to use a routine — say `expint_E1` — in her code should proceed as follows.

1. Add package **expint** to the `Imports` and `LinkingTo` directives of the 'DESCRIPTION' file of **pkg**;
2. Add an entry '`import(expint)`' in the 'NAMESPACE' file of **pkg**;
3. Define the routine with a call to `R_GetCCallable` in the initialization routine `R_init_pkg` of **pkg** (R Core Team, 2016, Section 5.4). For the current example, the file 'src/init.c' of **pkg** would contain the following code:

```
void R_init_pkg(DllInfo *dll)
{
    R_registerRoutines( /* native routine registration */ );

    pkg_expint_E1 = (double(*)(double,int,int))
                    R_GetCCallable("expint", "expint_E1");
}
```

4. Define a native routine interface that will call `expint_E1`, say `pkg_expint_E1` to avoid any name clash, in 'src/init.c' as follows:

```
double(*pkg_expint_E1)(double,int);
```

5. Declare the routine in a header file of **pkg** with the keyword `extern` to expose the interface to all routines of the package. In our example, file 'src/pkg.h' would contain:

```
extern double(*pkg_expint_E1)(double,int);
```

6. Include the package header file 'pkg.h' in any C file making use of routine `pkg_expint_E1`.

To help developers get started, **expint** ships with a complete test package implementing the above; see the 'example_API' sub-directory in the installation directory. This test package uses the `.External` R to C interface and, as a bonus, shows how to vectorize an R function on the C side (the code for this being mostly derived from base R).

There are various ways to define a package API. The approach described above was derived from package **zoo** (Zeileis and Grothendieck, 2005). Package **xts** (Ryan and Ulrich, 2014) — and probably a few others on CRAN — draws from **Matrix** (Bates and Maechler, 2016) to propose a somewhat simpler approach where the API exposes routines that can be used directly in a package. However, the provided header file can be included only once in a package, otherwise one gets '`duplicate symbols`' errors at link time. This constraint does no show in the example provided with **xts** or in packages **RcppXts** (Eddelbuettel, 2013) and **TTR** (Ulrich, 2016) that link to it (the only two at the time of writing). A way around the issue is to define a native routine calling the routines exposed in the API. In this scenario, tests we conducted proved the approach we retained to be up to 10% faster most of the time.

6 Implementation details

As already stated, the C routines mentioned in section 5 are derived from code in the GNU Scientific Library (Galassi et al., 2009).

For exponential integrals, the main routine `expint_E1` computes $E_1(x)$ using Chebyshev expansions (Gil et al., 2007, chapter 3). Routine `expint_E2` computes $E_2(x)$ using `expint_E1` with relation (4) for $x < 100$, and using the asymptotic expression (5) otherwise. Routine `expint_En` simply relies on `gamma_inc` to compute $E_n(x)$ for $n > 2$ through relation (3).

For the sake of providing routines that better fit within the R ecosystem and coding style, we made the following changes to the original GSL code:

1. routines now compute a single value and return their result by value;

2. accordingly, calculation of the approximation error was dropped in all routines;

3. most importantly, `gamma_inc` does not compute $\Gamma(a, x)$ for $a > 0$ with (7) using the GSL routines, but rather using routines `gammafn` and `pgamma` part of the R API.

The following illustrates the last point.

```
> options(digits = 20)
> gammainc(1.2, 3)
[1] 0.065421428091009217742
> gamma(1.2) * pgamma(3, 1.2, 1, lower = FALSE)
[1] 0.065421428091009217742
```

7 Alternative packages

The Comprehensive R Archive Network[1] (CRAN) contains a number of packages with features overlapping **expint**. We review the similarities and differences here.

The closest package in functionality is **gsl** (Hankin, 2006). This package is an R wrapper for the special functions and quasi random number generators of the GNU Scientific Library. As such, it provides access to basically the same C code as used in **expint**. Apart from the changes to the GSL code mentioned in section 6, the main difference between the two packages is that **gsl** requires that the GSL be installed on one's system, whereas **expint** is a regular, free standing R package.

Package **VGAM** (Yee, 2015) is a large, high quality package that provides functions to compute the exponential integral $\mathrm{Ei}(x)$ for real values, as well as $e^{-x}\,\mathrm{Ei}(x)$ and $E_1(x)$ and their derivatives (up to the third derivative). Functions `expint`, `expexpint` and `expint.E1` are wrappers to the Netlib[2] FORTRAN subroutines in file `ei.f`. **VGAM** does not provide an API to its C routines.

Package **pracma** (Borchers, 2016) provides a large number of functions from numerical analysis, linear algebra, numerical optimization, differential equations and special functions. Its versions of `expint`, `expint_E1`, `expint_Ei` and `gammainc` are entirely written in R with perhaps less focus on numerical accuracy than the GSL and Netlib implementations. The version of `gammainc` only supports positive values of a.

Package **frmqa** (Tran, 2012) has a function `gamma_inc_err` that computes the incomplete gamma function using the incomplete Laplace integral, but it is only valid for $a = j + \frac{1}{2}$, $j = 0, 1, 2, \ldots$.

Package **zipfR** (Evert and Baroni, 2007) introduces a set of functions to compute various quantities related to the gamma and incomplete gamma functions, but these are essentially wrappers around the base R functions `gamma` and `pgamma` with no new functionalities.

[1] https://cran.r-project.org
[2] http://www.netlib.org

8 Examples

We tabulate the values of $E_n(x)$ for $x = 1.275, 10, 12.3$ and $n = 1, 2, \ldots, 10$ as found in examples 4–6 of Abramowitz and Stegun (1972, section 5.3).

```
> x <- c(1.275, 10, 12.3)
> n <- 1:10
> structure(t(outer(x, n, expint)),
+           dimnames = list(n, paste("x =", x)))
    x = 1.275       x = 10     x = 12.3
1  0.14080993 4.156969e-06 3.439534e-07
2  0.09989831 3.830240e-06 3.211177e-07
3  0.07603031 3.548763e-06 3.009983e-07
4  0.06083077 3.304101e-06 2.831550e-07
5  0.05046793 3.089729e-06 2.672346e-07
6  0.04301687 2.900528e-06 2.529517e-07
7  0.03743074 2.732441e-06 2.400730e-07
8  0.03310097 2.582217e-06 2.284066e-07
9  0.02965340 2.447221e-06 2.177930e-07
10 0.02684699 2.325303e-06 2.080990e-07
```

We also tabulate the values of $\Gamma(a, x)$ for $a = -1.5, -1, -0.5, 1$ and $x = 1, 2, \ldots, 10$.

```
> a <- c(-1.5, -1, -0.5, 1)
> x <- 1:10
> structure(t(outer(a, x, gammainc)),
+           dimnames = list(x, paste("a =", a)))
       a = -1.5       a = -1     a = -0.5        a = 1
1  1.264878e-01 1.484955e-01 1.781477e-01 3.678794e-01
2  1.183299e-02 1.876713e-02 3.009876e-02 1.353353e-01
3  1.870260e-03 3.547308e-03 6.776136e-03 4.978707e-02
4  3.706365e-04 7.995573e-04 1.733500e-03 1.831564e-02
5  8.350921e-05 1.992938e-04 4.773965e-04 6.737947e-03
6  2.045031e-05 5.304291e-05 1.379823e-04 2.478752e-03
7  5.310564e-06 1.478712e-05 4.127115e-05 9.118820e-04
8  1.440569e-06 4.267206e-06 1.266464e-05 3.354626e-04
9  4.042025e-07 1.264846e-06 3.964430e-06 1.234098e-04
10 1.165117e-07 3.830240e-07 1.260904e-06 4.539993e-05
```

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private communication. Joshua Ulrich provided a fix to the API infrastructure to avoid duplicated symbols that was implemented in version 0.1-6 of the package.

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