log1pmx(), bd0(), stirlerr() – Computing Poisson, Binomial, Gamma Probabilities in R

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Abstract

The auxiliary function log1pmx() ("log 1 **p**lus **m**inus x"), had been introduced when R's `pgamma()` (incomplete Γ function) had been numerically improved by Morten Welinder's contribution to R's PR#7307, in Jan. 2005[1], it is mathematically defined as $\text{log1pmx}(x) := \log(1 + x) - x$ and for numerical evaluation, suffers from two levels of cancellations for small x, i.e., using log1p(x) for $\log(1 + x)$ is not sufficient.

In 2000 already, Catherine Loader's contributions for more accurate computation of binomial, Poisson and negative binomial probabilities, Loader (2000), had introduced auxiliary functions `bd0()` and `stirlerr()`, see below.

Much later, in R's PR#15628, in Jan. 2014[2], Welinder noticed that in spite of Loader's improvements, Poisson probabilities were not perfectly accurate (only ca. 13 accurate digits instead of $15.6 \approx \log_{10}(2^{52})$), relating the problem to somewhat imperfect computations in `bd0()`, which he proposed to address using `log1pmx()` on one hand, and additionally addressing cancellation by using *two* double precision numbers to store the result (his proposal of an `ebd0()` function).

Here, I address the problem of providing more accurate `bd0()` (and `stirlerr()` as well), applying Welinder's proposal to use log1pmx(), but otherwise diverging from the proposal.

1 Introduction

According to R's reference documentation, `help(dbinom)`, the binomial (point-mass) probabilities of the binomial distribution with `size` $= n$ and `prob` $= p$ has "density" (point probabilities)

$$p(x) := p(x; n, p) := \binom{n}{x} p^x (1 - p)^{n-x} \;, \tag{1}$$

for $x = 0, \ldots, n$, and these are (in Rfunction `dbinom()`) computed via Loader's algorithm (Loader (2000)) which had improved accuracy considerably, also for R's internal `dpois_raw()` function which is used further directly in `dpois()`, `dnbinom()`, `dgamma()`, the non-central `dbeta()` and `dchisq()` and even the *cumulative* $\Gamma()$ probabilities `pgamma()` and hence indirectly e.g., for cumulative central and non-central chisquare probabilities (`pchisq()`).

Loader noticed that for large n, the usual way to compute $p(x; n, p)$ via its logarithm $\log(p(x; n, p)) = \log(n!) - \log(x!) - \log((n-x)!) + x \log(p) + (n-x) \log(1-p)$ was inaccurate,

[1] `https://bugs.R-project.org/show_bug.cgi?id=7307#c6`
[2] `https://bugs.r-project.org/show_bug.cgi?id=15628`

even when accurate $\log\Gamma(x) =$ `lgamma(x)` values are available to get $\log(x!) = \log\Gamma(x+1)$, e.g., for $x = 10^6$, $n = 2 \times 10^6$, $p = 1/2$, about 7 digits accuracy were lost from cancellation (in substraction of the log factorials).

Instead, she wrote

$$p(x; n, p) = p(x; n, \frac{x}{n}) \cdot e^{-D(x;n,p)}, \tag{2}$$

where the "Deviance" $D(.)$ is defined as

$$\begin{aligned} D(x; n, p) &= \log p(x; n, \frac{x}{n}) - \log p(x; n, p) \\ &= x \log\left(\frac{x}{np}\right) + (n-x)\log\left(\frac{n-x}{n(1-p)}\right), \end{aligned} \tag{3}$$

and to avoid cancellation, $D()$ has to be computed somewhat differently, namely – correcting notation wrt the original – using a *two*-argument version $D_0()$:

$$\begin{aligned} D(x; n, p) &= np\tilde{D}_0\left(\frac{x}{np}\right) + nq\tilde{D}_0\left(\frac{n-x}{nq}\right) \\ &= D_0(x, np) + D_0(n-x, nq), \end{aligned} \tag{4}$$

where $q := 1 - p$ and

$$\tilde{D}_0(r) := r\log(r) + 1 - r \quad \text{and} \tag{5}$$

$$D_0(x, M) := M \cdot \tilde{D}_0(x/M) \tag{6}$$

$$= M \cdot \left(\frac{x}{M}\log\left(\frac{x}{M}\right) + 1 - \frac{x}{M}\right) = x\log\left(\frac{x}{M}\right) + M - x \tag{7}$$

Note that since $\lim_{x\downarrow 0} x \log x = 0$, setting

$$\begin{aligned} \tilde{D}_0(0) &:= 1 \text{ and} \\ D_0(0, M) &:= M\tilde{D}_0(0) = M \cdot 1 = M \end{aligned} \tag{8}$$

defines $D_0(x, M)$ for all $x \geq 0$, $M > 0$.

The careful C function implementation of $D_0(x, M)$ is called `bd0(x, np)` in Loader's C code and now R's Mathlib ((lib)Rmath) at `https://svn.r-project.org/R/trunk/src/nmath/bd0.c`, mirrored, e.g., at Winston Chen's github mirror[3]. In 2014, Morten Welinder suggested in R's PR#15628[4] that the current `bd0()` implementation is still inaccurate in some regions (mostly *not* in the one it has been carefully implemented to be accurate, i.e., when $x \approx M$) notably for computing Poisson probabilities, `dpois()` in R; see more below.

Evaluating of $p(x; n, p)$ in (1) and (2), in addition to $D(x; n, p)$ in (4) also needs $p(x; n, \frac{x}{n})$ where in turn, the Stirling De Moivre series is used:

$$\log n! = \frac{1}{2}\log(2\pi n) + n\log(n) - n + \delta(n), \quad \text{where the "Stirling error" } \delta(n) \text{ is} \tag{9}$$

$$\delta(n) := \log n! - \frac{1}{2}\log(2\pi n) - n\log(n) + n = \tag{10}$$

$$= \frac{1}{12n} - \frac{1}{360n^3} + \frac{1}{1260n^5} - \frac{1}{1680n^7} + \frac{1}{1188n^9} + O(n^{-11}). \tag{11}$$

[3]`https://github.com/wch/r-source/blob/trunk/src/nmath/bd0.c`

[4]`https://bugs.r-project.org/show_bug.cgi?id=15628`

See appendix C how $\delta(n) \equiv$stirlerr(n) is computed and implemented in the C code of R, and can be improved.

Note that for the binomial, x is an integer in $\{0, 1, \ldots, n\}$ and $M = np \geq 0$, but the formulas (6), (7) for $D_0(x, M)$ apply and are needed, e.g., for pgamma() computations for general non-negative $(x, M > 0)$ where even the $x = 0$ case is well defined, see (8) above.

Summarizing, using (1), (6), (7), the binomial probabilities in R, dbinom(x, n,p) have been computed as

$$p(x; n, p) = p(x; n, \frac{x}{n}) \cdot e^{-D(x;n,p)} = \tag{12}$$

$$= \sqrt{\frac{n}{2\pi x(n-x)}} e^{\delta(n)-\delta(x)-\delta(n-x)}, \tag{13}$$

the second line being eq. (5) of Loader which is derived by using Stirling's (9) three times, viz. for n, x, and $n - x$, and noticing that many log terms cancel and the three $\log(2\pi *)/2$ terms simplify to $\log(\frac{n}{2\pi x(n-x)})/2$.

Further, Loader showed that such a saddle point approach is needed for Poisson probabilities, as well, where

$$p_\lambda(x) = e^{-\lambda} \frac{\lambda^x}{x!} \tag{14}$$

$$\log p_\lambda(x) = -\lambda + x \log \lambda \qquad \underbrace{- \log(x!)}_{\log(1/\sqrt{2\pi x}) - (x \log x - x + \delta(x))}$$

$$= \log \frac{1}{\sqrt{2\pi x}} - x \log \frac{x}{\lambda} + x - \lambda - \delta(x), \tag{15}$$

is re-expressed using $\delta(x)$ and from (7) $D_0(x, \lambda)$ as

$$p_\lambda(x) = \frac{1}{\sqrt{2\pi x}} e^{-\delta(x) - D_0(x,\lambda)} \tag{16}$$

Also, negative binomial probabilities, dnbinom(), ... TODO ......

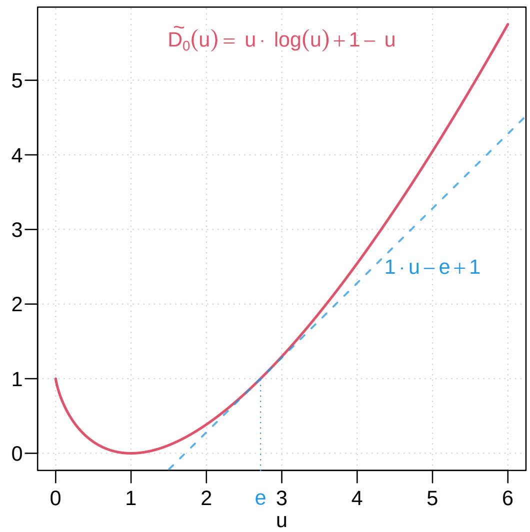
Even for the t_ν density, dt(), ...
...but there have a direct approximations in package **DPQ**, currently functions c_dt(nu) and even more promisingly, lb_chi(nu). .... TODO ......

2 Loader's "Binomial Deviance" $D_0(x, M) =$ bd0(x, M)

Loader's "*Binomial Deviance*" function $D_0(x, M) =$ bd0(x, M) has been defined for $x, M > 0$ where the limit $x \to 0$ is allowed (even though not implemented in the original bd0()), here repeated from (6) :

$$D_0(x, M) := M \cdot \tilde{D}_0(\frac{x}{M}), \quad \text{where}$$
$$\tilde{D}_0(u) := u \log(u) + 1 - u = u(\log(u) - 1) + 1.$$

Note the graph of $\tilde{D}_0(u)$,



has a double zero at $u = 1$, such that for large M and $x \approx M$, i.e., $\frac{x}{M} \approx 1$, the direct computation of $D_0(x, M) = M \cdot \tilde{D}_0\bigl(\frac{x}{M}\bigr)$ is numerically problematic. Further,

$$D_0(x, M) = M \cdot \Bigl(\frac{x}{M}(\log(\frac{x}{M}) - 1) + 1\Bigr) = x\log(\frac{x}{M}) - x + M. \tag{17}$$

We can rewrite this, originally by e-mail from Martyn Plummer, then also indirectly from Morten Welinder's mentioning of `log1pmx()` in his PR#15628 notably for the important situation when $|x - M| \ll M$. Setting $t := (x - M)/M$, i.e., $|t| \ll 1$ for that situation, or equivalently, $\frac{x}{M} = 1 + t$. Using t,

$$t := \frac{x - M}{M} \tag{18}$$

$$\begin{aligned} D_0(x, M) &= \overbrace{M \cdot (1 + t)}^{x}\log(1 + t) - \overbrace{t \cdot M}^{x-M} = M \cdot \bigl((t + 1)\log(1 + t) - t\bigr) = \\ &= M \cdot p_1 l_1(t), \end{aligned} \tag{19}$$

where

$$\begin{aligned} p_1 l_1(t) &:= (t + 1)\log(1 + t) - t = \frac{t^2}{2} - \frac{t^3}{6} \pm \cdots, & (20) \\ &= (\log(1 + t) - t) + t \cdot \log(1 + t) \\ &= \mathrm{log1pmx}(t) + t \cdot \mathrm{log1p}(t) & (21) \end{aligned}$$

where

$$\mathrm{log1pmx}(x) := \log(1 + x) - x \approx -x^2/2 + x^3/3 - x^4/4 \pm \ldots, \tag{22}$$

and the Taylor series expansions for $\mathrm{log1pmx}(t)$ and $p_1 l_1(t)$ are useful for small $|t|$,

$$\begin{aligned} p_1 l_1(t) &= \frac{t^2}{2} - \frac{t^3}{6} + \frac{t^4}{12} \pm \cdots = \sum_{n=2}^{\infty} \frac{(-t)^n}{n(n-1)} = \frac{t^2}{2}\sum_{n=2}^{\infty}\frac{(-t)^{n-2}}{n(n-1)/2} = \frac{t^2}{2}\sum_{n=0}^{\infty}\frac{(-t)^n}{\binom{n+2}{2}} = & (23) \\ &= \frac{t^2}{2}\Bigl(1 - t\bigl(\frac{1}{3} - t(\frac{1}{6} - t(\frac{1}{10} - t(\frac{1}{15} - \cdots))))\Bigr), & (24) \end{aligned}$$

which we provide in **DPQ** via function `p1l1ser(t, k)` getting the first k terms, and the corresponding series approximation for

$$D_0(x, M) = \lim_{k \to \infty} \mathrm{p1l1ser}\Big(\frac{x - M}{M},\ k,\ F = \frac{(x - M)^2}{M}\Big), \tag{25}$$

where the approximation of course uses a finite k instead of the limit $k \to \infty$.

This Taylor series expansion is useful and nice, but may not even be needed typically, as both utility functions $\mathrm{log1pmx}(t)$ and $\mathrm{log1p}(t)$ are available implemented to be fully accurate for small t, $t \ll 1$, and (21), indeed, with $t = (x - M)/M$ the evaluation of

$$D_0(x, M) = M \cdot p_1 l_1(t) = M \cdot \big(\mathrm{log1pmx}(t) + t \cdot \mathrm{log1p}(t)\big), \tag{26}$$

seems quite accurate already on a wide range of (x, M) values.

```
> par(mfcol=1:2, mar = 0.1 + c(2.5, 3, 1, 2), mgp = c(1.5, 0.6, 0), las=1)
> p.p1l1(-7/8, 2, ylim = c(-1,2))
> zoomTo <- function(x,y=x, tx,ty){ arrows(x,-y, tx, ty)
+                                   text(x,-y, "zoom in", adj=c(1/3,9/8)) }
> zoomTo0 <- function(x,y=x) zoomTo(x,y, 0,0)
> zoomTo0(.3)
> p.p1l1(-1e-4, 1.5e-4, ylim=1e-8*c(-.6, 1), do.leg=FALSE)
```

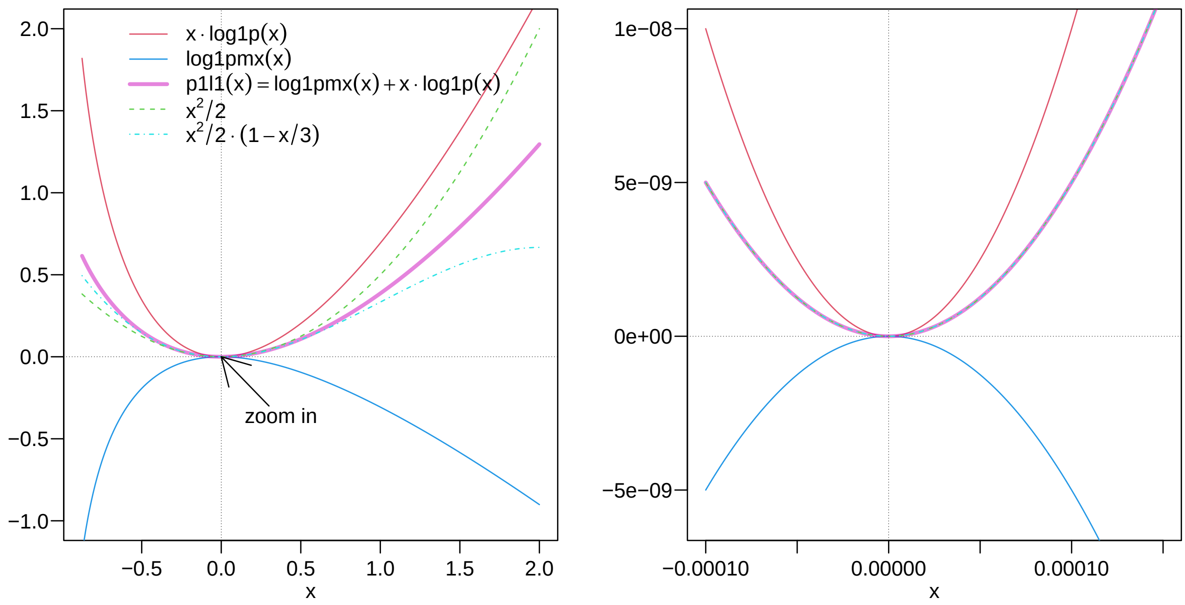


Figure 1: $p_1 l_1(t) =$ `p1l1()` and its constituents, $x * \mathrm{log1p}(x)$ and $\mathrm{log1pmx}() =$ `log1pmx()`, with Rfunctions from our **DPQ** package. On the right, zoomed in 4 and 8 orders of magnitude, where the Taylor approximations $x^2/2$ and $x^2/2 - x^3/6$ are visually already perfect.

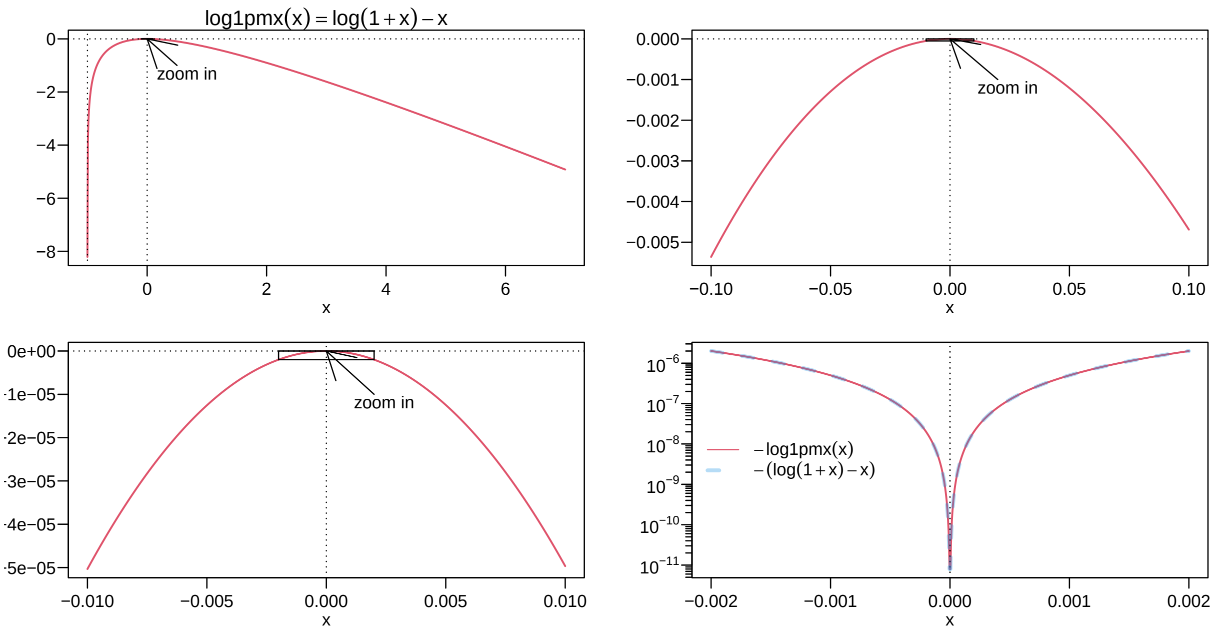
Note that $x * \mathrm{log1p}(x)$ and $\mathrm{log1pmx}()$ have different signs, but also note that for small $|x|$, are well approximated by x^2 and $-x^2/2$, so their sum $p_1 l_1(x) = \mathrm{log1pmx}(x) + x \cdot \mathrm{log1p}(x)$ is approximately $x^2/2$ *and* numerically computing $x^2 - x^2/2$ should only lose 1 or 2 bits of precision.

A Accuracy of log1pmx(x) Computations

As we've seen, the "binomial deviance" function $D_0(x, M)$ = `bd0(x, M)` is crucial for accurate (saddlepoint) computations of binomial, Poisson, etc probabilities, and (at the end of section 2), one stable way to compute $D_0(x, M)$ is via (26), i.e., with $t = (x - M)/M$, to compute the sum of two terms $D_0(x, M) = M \cdot \big(\mathrm{log1pmx}(t) + t \cdot \mathrm{log1p}(t)\big)$.

Here, we look more closely at the computation of $\mathrm{log1pmx}(x) := \log(1 + x) - x$, at first visualizing the function, notably around $(0, 0)$ where numeric cancellations happen if no special care is taken.

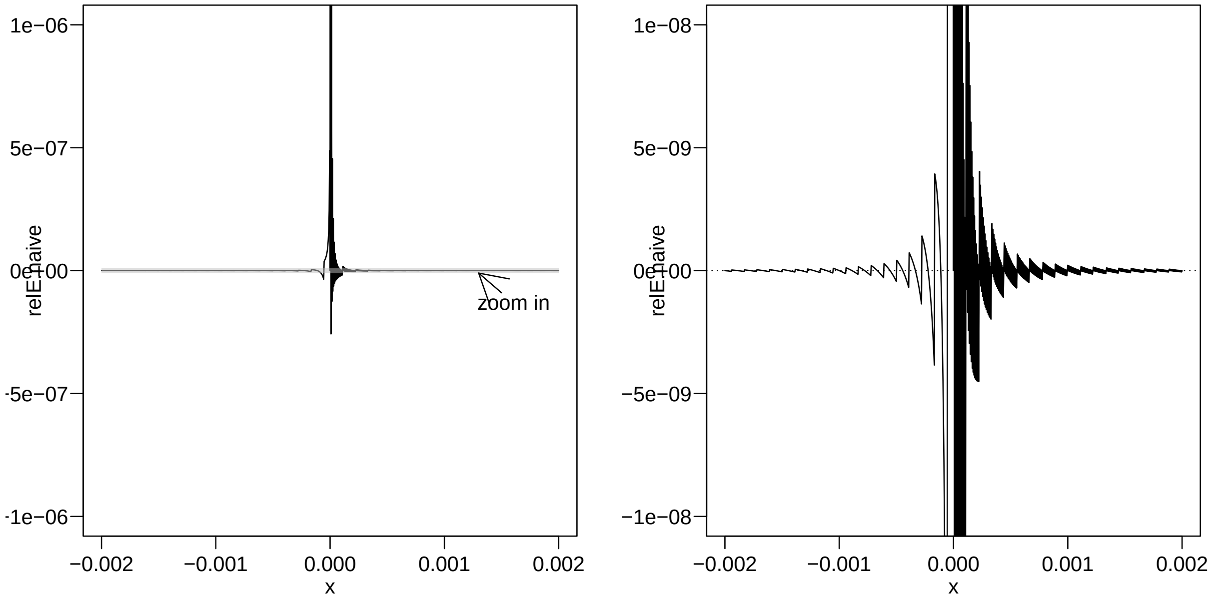
```
> lcurve <- function(Fn, a,b, ylab = "", lwd = 1.5, ...)
+     plot(Fn, a,b, n=1001, col=2, ylab=ylab, lwd=lwd, ...,
+          panel.last = abline(h=0, v=-1:0, lty=3))
> par(mfrow=c(2,2), mar = 0.1 + c(2.5, 3, 1, 2), mgp = c(1.5, 0.6, 0), las=1)
> lcurve(log1pmx, -.9999, 7, main=quote(log1pmx(x) == log(1+x)-x))
>                            rect(-.1,  log1pmx(-.1  ), .1   , 0); zoomTo0(1/2, 1)
> lcurve(log1pmx, -.1,  .1 ); rect(-.01, log1pmx(-.01 ), .01 , 0); zoomTo0(.02, .001)
> lcurve(log1pmx, -.01, .01); rect(-.002,log1pmx(-.002), .002, 0); zoomTo0(2e-3,1e-5)
> lcurve(function(x) -log1pmx(x), -.002, .002, log="y", yaxt="n") -> l1r
> sfsmisc::eaxis(2); abline(v=0, lty=3)
> d1r <- cbind(as.data.frame(l1r), y.naive = with(l1r, -(log(1+x)-x)))
> c4 <- adjustcolor(4, 1/3)
> lines(y.naive ~ x, data=d1r, col=c4, lwd=3, lty=2)
> legend("left", legend=expression(- log1pmx(x), -(log(1+x)-x)),
+         col=c(palette()[2],c4), lwd=c(1,3), lty=1:2, bty="n")
```



The accuracy of our `log1pmx()` is already vastly better than the naive $\log(1 + x) - x$ computation:

```
> par(mfrow=1:2, mar = 0.1 + c(2.5, 3, 1, 2), mgp = c(1.5, 0.6, 0), las=1)
> d1r[, "relE.naive"] <- with(d1r, sfsmisc::relErrV(y, y.naive))
> plot(relE.naive ~ x, data=d1r, type="l", ylim = c(-1,1)*1e-6)
> y2 <- 1e-8
> rect(-.002, -y2, .002, y2, col=adjustcolor("gray",1/2), border="transparent")
```

```
> zoomTo(15e-4, 9*y2, 13e-4, -y2)
> plot(relE.naive ~ x, data=d1r, type="l", ylim = c(-1,1)*y2); abline(h=0,lty=3)
```



Now, we explore the accuracy achieved with R's, i.e. Welinder's algorithm, which uses relatively few terms ao continued-fraction representation of the Taylor series of log1pmx(x), using package **Rmpfr** and high precision arithmetic. see '`../tests/dnbinom-tst.R`', `2b: log1pmx()`. From there, it seems that the (hardcoded currently in R's '`pgamma.c`' as `double minLog1Value = -0.79149064` could or should (?) be changed to around -0.7 or e.g., -0.66.

In **DPQ**'s `log1pmx()` it is the argument `minL1 = -0.79149064`, there' a switch constant eps2, (hardwired in current Rto `1e-2`, i.e., `eps2 = 0.02`) to switch from an explicit 5-term formula to the full `logcf()` based procedure. In **DPQ**, we already use `eps2 = 0.01` as default. Note that this does *not* influence the choice of `minL1` as long as `eps2` (order of 0.01) is far from the range in which we choose `minL1` ($[-0.85, -0.4]$).
((MM: Still: can we prove that 0.01 is "uniformly" better than 0.02 ??))

A.1 Testing `dpois_raw()` / `dpois()` Poisson probabilities

Testing the Poisson probabilities ('density') with several versions of bd0(), ebd0() and the direct formula where more appropriate (non-log case, Look at examples in '`"../man/dgamma-utils.Rd"`' and then also
`/u/maechler/R/MM/NUMERICS/dpq-functions/15628-dpois_raw_accuracy.R` .

B Accuracy of $p_1l_1(t)$ Computations

Loader's "Binomial Deviance" $D_0(x, M)$ = `bd0(x, M)` function can also be re-expressed (mathematically) as $bd0(x, M) = M * p1l1((x - M)/M)$ where we look into providing numerically stable formula for $p1l1(t)$ as its mathematical formula $p1l1(t) = (t+1)\log(1+t) - t$ suffers from cancellation for small $|t|$ even when `log1p(t)` is used instead of `log(1+t)`; see the derivations (19), (20), and (22) above, and the Taylor series expansion (23) which we provide in our Rfunctions `p1l1()`, and `p1l1ser`, respectively.

Using a hybrid implementation, `p1l1()` uses a direct formula, now the stable one in `p1l1p()`, for $|t| > c$ and a series approximation for $|t| \leq c$ for some cutoff c.

NB: The re-expression via `log1pmx()` is almost perfect; it fixes the cancellation problem entirely (and exposes the fact that `log1pmx()`'s internal cutoff seems sub optimal.

TODO — very unfinished. How much more here?

For now, look at the examples in `?p1l1`, or even run `example(p1l1)`.

C Accuracy of `stirlerr(x)`$= \delta(x)$ Computations

Note that the "Stirling error", $\delta(x) \equiv$`stirlerr(x)`, $\delta(x) := \log x! - \frac{1}{2}\log(2\pi x) - x\log(x) + x$ by Stirling's formula is $\delta(x) = \frac{1}{12x} - \frac{1}{360x^3} + \frac{1}{1260x^5} - \frac{1}{1680x^7} + \frac{1}{1188x^9} + O(x^{-11})$, see (10).

A C code implementation had been provided by Loader and for years now in R's Mathlib at https://svn.r-project.org/R/trunk/src/nmath/stirlerr.c. mirrored, e.g., at https://github.com/wch/r-source/blob/trunk/src/nmath/stirlerr.c

TODO:

Look at examples in '`../tests/stirlerr-tst.R`' to show the small accuracy loss with Loader's defaults (for the cut offs of the number of terms used) and also how we explore improving these defaults to improve accuracy.

References

Loader, C. (2000). Fast and accurate computation of binomial probabilities. Technical report, Lucent; Murray Hill, NJ USA.