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)

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

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* Γ() 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

$$p(x; n, p) = p(x; n, \frac{x}{n}) \cdot e^{-D(x;n,p)}, \tag{1}$$

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

$$\begin{aligned} D(x; n, p) &= \log p(x; n, \frac{x}{n}) - \log p(x; n, p) \\ &= x \log\big(\frac{x}{np}\big) + (n - x) \log\big(\frac{n - x}{n(1 - p)}\big), \end{aligned} \tag{2}$$

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

$$\begin{aligned} D(x; n, p) &= np\tilde{D}_0\big(\frac{x}{np}\big) + nq\tilde{D}_0\big(\frac{n - x}{nq}\big) \\ &= D_0(x, np) + D_0(n - x, nq), \end{aligned} \tag{3}$$

where $q := 1 - p$ and

$$\tilde{D}_0(r) := r \log(r) + 1 - r \quad \text{and} \tag{4}$$

$$D_0(x, M) := M \cdot \tilde{D}_0(x/M) \tag{5}$$

$$= M \cdot \Big(\frac{x}{M} \log\big(\frac{x}{M}\big) + 1 - \frac{x}{M}\Big) = x \log\big(\frac{x}{M}\big) + M - x \tag{6}$$

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

$$\begin{aligned} \tilde{D}_0(0) &:= 1 \text{ and} \\ D_0(0, M) &:= M\tilde{D}_0(0) = M \cdot 1 = M \end{aligned} \tag{7}$$

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), in addition to $D(x; n, p)$ in (3) also needs $p(x; n, \frac{x}{n})$ where in turn, the Stirling De Moivre series is used:

$$\log n! = \frac{1}{2}\log(2\pi n) + n\log(n) - n + \delta(n), \quad \text{where the "Stirling error" } \delta(n) \text{ is} \tag{8}$$

$$\delta(n) := \log n! - \frac{1}{2}\log(2\pi n) - n\log(n) + n = \tag{9}$$

$$= \frac{1}{12n} - \frac{1}{360n^3} + \frac{1}{1260n^5} - \frac{1}{1680n^7} + \frac{1}{1188n^9} + O(n^{-11}). \tag{10}$$

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

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

Note that $\delta(n) \equiv$ `stirlerr(n)` in the C code provided by Loader and now in R's Mathlib at https://svn.r-project.org/R/trunk/src/nmath/stirlerr.c.

Note that for the binomial, x is an integer in $\{0, 1, \dots, n\}$ and $M = np \geq 0$, but the formulas (5), (6) for $D_0(x, M)$ apply and are needed, e.g., for `pgamma()` computations for general non-negative $(x, M > 0)$ where even $x = 0$ is well defined, see (7) above.

Further (see Loader), such a saddle point approach is needed for Poisson probabilities, as well, where

$$p_\lambda(x) = e^{-\lambda}\frac{\lambda^x}{x!} \tag{11}$$

$$\begin{aligned}\log p_\lambda(x) &= -\lambda + x\log\lambda \underbrace{\qquad - \log(x!)}_{\log(1/\sqrt{2\pi x}) - (x\log x - x + \delta(x))} \\ &= \log\frac{1}{\sqrt{2\pi x}} - x\log\frac{x}{\lambda} + x - \lambda - \delta(x),\end{aligned} \tag{12}$$

is re-expressed using $\delta(x)$ and from (6) $D_0(x, \lambda)$ as

$$p_\lambda(x) = \frac{1}{\sqrt{2\pi x}} e^{-\delta(x) - D_0(x,\lambda)} \tag{13}$$

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

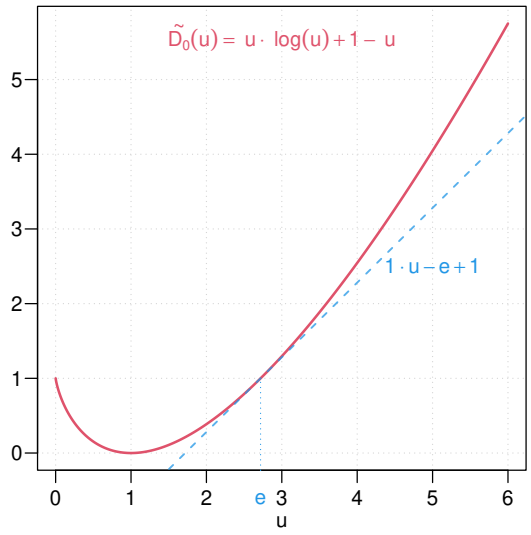
Even for the t_ν density, `dt()`, ...
... but there have a direct approximations in package **DPQ**, currently functions `c_dt(nu)` and even more promisingly, `lb_chi(nu)`. ..... TODO .....

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 (5) :

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

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 $D_0(x, M) = M \cdot \tilde{D}_0\big(\frac{x}{M}\big)$ is numerically problematic. Further,

$$D_0(x, M) = M \cdot \big(\frac{x}{M}(\log(\frac{x}{M}) - 1) + 1\big) = x \log(\frac{x}{M}) - x + M. \tag{14}$$

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,

$$t := \frac{x - M}{M} \tag{15}$$

$$D_0(x, M) = \overbrace{M \cdot (1 + t)}^{x} \log(1 + t) - \overbrace{t \cdot M}^{x-M} = M \cdot \big((t + 1) \log(1 + t) - t\big) =$$
$$= M \cdot p_1 l_1(t), \tag{16}$$

where

$$p_1 l_1(t) := (t + 1) \log(1 + t) - t = \frac{t^2}{2} - \frac{t^3}{6} \pm \cdots, \tag{17}$$
$$= (\log(1 + t) - t) + t \cdot \log(1 + t)$$
$$= \mathrm{log1pmx}(t) + t \cdot \mathrm{log1p}(t) \tag{18}$$

where

$$\mathrm{log1pmx}(x) := \log(1 + x) - x \approx -x^2/2 + x^3/3 - x^4/4 \pm \ldots, \tag{19}$$

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

$$p_1 l_1(t) = \frac{t^2}{2} - \frac{t^3}{6} + \frac{t^4}{12} \pm \cdots = \sum_{n=2}^{\infty} \frac{(-t)^n}{n(n-1)} = \frac{t^2}{2} \sum_{n=2}^{\infty} \frac{(-t)^{n-2}}{n(n-1)/2} = \frac{t^2}{2} \sum_{n=0}^{\infty} \frac{(-t)^n}{\binom{n+2}{2}} = \tag{20}$$
$$= \frac{t^2}{2}\big(1 - t\big(\frac{1}{3} - t\big(\frac{1}{6} - t\big(\frac{1}{10} - t\big(\frac{1}{15} - \cdots\big)\big)\big)\big)\big), \tag{21}$$

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

$$D_0(x, M) = \lim_{k \to \infty} \mathrm{p1l1ser}\big(\frac{x - M}{M},\ k,\ F = \frac{(x - M)^2}{M}\big), \tag{22}$$

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 (18), indeed, with $t = (x - M)/M$ the evaluation of

$$D_0(x, M) = M \cdot p_1 l_1(t) = M \cdot \big(\mathrm{log1pmx}(t) + t \cdot \mathrm{log1p}(t)\big), \tag{23}$$

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

Note that $x * \mathrm{log1p}(x)$ and 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.

```
> par(mfcol=1:2, mar = 0.1 + c(2.5, 3, 1, 2), mgp = c(1.5, 0.6, 0), las=1)
> p.pl1l(-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.pl1l(-1e-4, 1.5e-4, ylim=1e-8*c(-.6, 1), do.leg=FALSE)
```

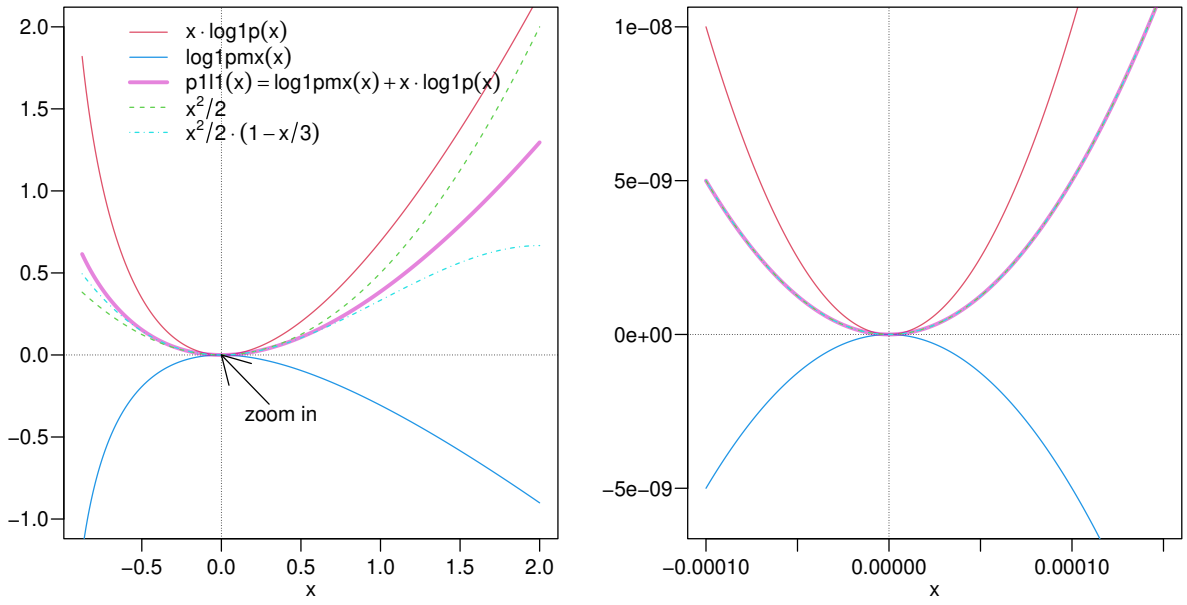


Figure 1: $p_1 l_1(t) =$ `p1l1()` and its constituents, $x * \mathrm{log1p}(x)$ and $\mathrm{log1pmx}() =$ `log1pmx()`, with Rfunctions from our **DPQ** package. On the right, zoomed in 4 and 8 orders of magnitude, where the Taylor approximations $x^2/2$ and $x^2/2 - x^3/6$ are visually already perfect.

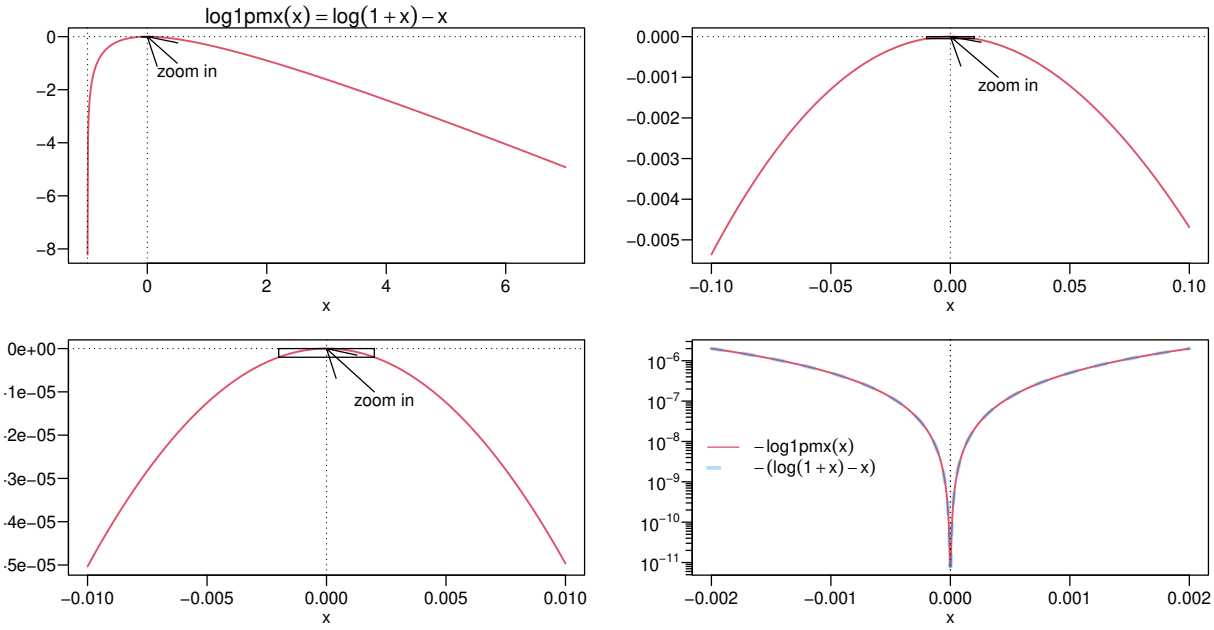
3 Appendix A: Accuracy of log1pmx(x) Computations

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 (23), 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.

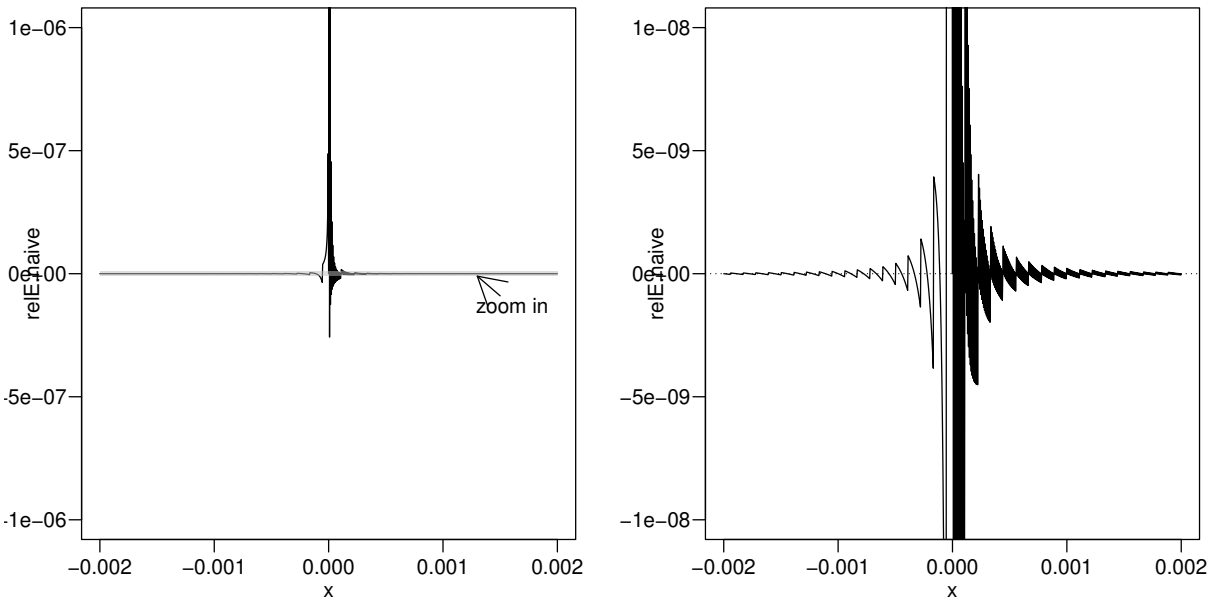
```
> lcurve <- function(Fn, a,b, ylab = "", lwd = 1.5, ...)
+     plot(Fn, a,b, n=1001, col=2, ylab=ylab, lwd=lwd, ...,
+          panel.last = abline(h=0, v=-1:0, lty=3))
> par(mfrow=c(2,2), mar = 0.1 + c(2.5, 3, 1, 2), mgp = c(1.5, 0.6, 0), las=1)
> lcurve(log1pmx, -.9999, 7, main=quote(log1pmx(x) == 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(\(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.

4 Appendix B: Accuracy of $p_1 l_1(t)$ Computations

References

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