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

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Abstract

The auxiliary function $\log 1 \text{pmx}()$ (" $\log 1 \text{ plus minus x}$ "), had been introduced by Morten Welinder in his proposal to improve R's pgamma() (incomplete Γ function) numerically, in R's PR#7307 comment #6¹, in Jan. 2005. log1pmx() has also been added to the R's C API Mathlib (aka libRmath, r-mathlib, or nmath) library in March 2005. It is defined as $\log 1 \text{pmx}(x) := \log(1+x) - x$ and for numerical evaluation, suffers from two levels of cancellations for small x, i.e., using $\log 1 \text{p(x)}$ 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. 2014², 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.

Notably, I noticed that ebd0() currently suffers from accuracy loss, when bd0(x,M) is large and $x/M \approx 1$.

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)

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

for x = 0, ..., n, and these are (in R function 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()

¹https://bugs.R-project.org/show_bug.cgi?id=7307#c6

²https://bugs.r-project.org/show_bug.cgi?id=15628

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, even when accurate $\log \Gamma(x) = \text{Igamma}(\mathbf{x})$ 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

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

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

$$D(x; n, p) = \log p(x; n, \frac{x}{n}) - \log p(x; n, p)$$

$$= x \log \left(\frac{x}{np}\right) + (n - x) \log \left(\frac{n - x}{n(1 - p)}\right), \tag{3}$$

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

$$D(x; n, p) = npd_0\left(\frac{x}{np}\right) + nqd_0\left(\frac{n-x}{nq}\right)$$
$$= D_0(x, np) + D_0(n-x, nq), \tag{4}$$

where q := 1 - p and

$$d_0(r) := r \log(r) + 1 - r \quad \text{and} \tag{5}$$

$$D_0(x, M) := M \cdot d_0(x/M)$$

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

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

$$d_0(0) := 1$$
 and
$$D_0(0, M) := M d_0(0) = M \cdot 1 = M$$
 (7)

defines $D_0(x, M)$ for all $x \ge 0$, 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 at https://svn.r-project.org/R/trunk/src/nmath/bd0.c, mirrored, e.g., at Winston Chen's github mirror³. In 2014, Morten Welinder suggested in R's PR#15628⁴ 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 in A.1 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:

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

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

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

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

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

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

Note that for the binomial, x is an integer in $\{0, 1, ..., n\}$ and $M = np \ge 0$, but the formulas around (6) 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 (7) above.

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

$$p(x; n, p) = p(x; n, \frac{x}{n}) \cdot e^{-D(x; n, p)} =$$
 (11)

$$= \sqrt{\frac{n}{2\pi x(n-x)}} e^{\delta(n)-\delta(x)-\delta(n-x)-D(x;n,p)}, \tag{12}$$

the second line from replacing $p(x; n, \frac{x}{n})$ by eq. (5) of Loader, derived by using Stirling's (8) 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

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

$$\log p_{\lambda}(x) = -\lambda + x \log \lambda \underbrace{-\log(x!)}_{\log(1/\sqrt{2\pi x}) - (x \log x - x + \delta(x))}$$
(13)

$$= \log \frac{1}{\sqrt{2\pi x}} - x \log \frac{x}{\lambda} + x - \lambda - \delta(x), \tag{14}$$

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

$$p_{\lambda}(x) = \frac{1}{\sqrt{2\pi x}} e^{-\delta(x) - D_0(x,\lambda)}$$
(15)

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

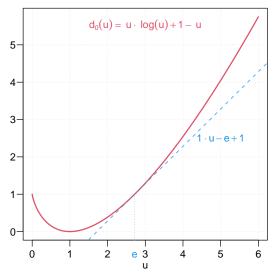
2 Loader's "Binomial Deviance" $D_0(x, M) = bd0(x, M)$

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), (6):

$$D_0(x, M) := M \cdot d_0(\frac{x}{M}), \text{ where}$$

 $d_0(u) := u \log(u) + 1 - u = u(\log(u) - 1) + 1.$

Note the graph of $d_0(u)$ (= $p_1l_1(u-1)$, see (18) below),



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 $D_0(x,M)=M\cdot d_0\left(\frac{x}{M}\right)$ is numerically problematic. Further,

$$D_0(x, M) = M \cdot \left(\frac{x}{M}(\log(\frac{x}{M}) - 1) + 1\right) = x \log(\frac{x}{M}) - x + M. \tag{16}$$

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, $\frac{x}{M} = 1 + t$.

With
$$t := \frac{x - M}{M}$$
 (17)

$$D_0(x, M) = \underbrace{M \cdot (1+t)}_{x} \log(1+t) - \underbrace{t \cdot M}_{x-M} = M \cdot ((t+1)\log(1+t) - t) =$$

$$= M \cdot p_1 l_1(t) \stackrel{!}{=} M \cdot d_0(t+1),$$
(18)

where

$$p_1 l_1(t) := (t+1)\log(1+t) - t = \frac{t^2}{2} - \frac{t^3}{6} \pm \cdots,$$

$$= (\log(1+t) - t) + t \cdot \log(1+t)$$
(19)

$$= \log_{1} \operatorname{pmx}(t) + t \cdot \log_{1} \operatorname{p}(t) \tag{20}$$

and

$$\log_{1} \text{pmx}(t) := \log_{1}(1+t) - t \quad \approx -t^{2}/2 + t^{3}/3 - t^{4}/4 \pm \dots$$
 (21)

The Taylor series expansions for log1pmx(t) and $p_1l_1(t)$ are useful for small |t|,

$$p_1 l_1(t) = \frac{t^2}{2} - \frac{t^3}{6} + \frac{t^4}{12} \pm \dots = \sum_{n=2}^{\infty} \frac{(-t)^n}{n(n-1)} = \frac{t^2}{2} \sum_{n=2}^{\infty} \frac{(-t)^{n-2}}{n(n-1)/2} = \frac{t^2}{2} \sum_{n=0}^{\infty} \frac{(-t)^n}{\binom{n+2}{2}} = \frac{t^2}{2} \left(1 - t\left(\frac{1}{3} - t\left(\frac{1}{6} - t\left(\frac{1}{10} - t\left(\frac{1}{15} - \dots\right)\right)\right)\right)\right), \tag{22}$$

which we provide in **DPQ** via function p111ser(t, k) getting the first k terms, and by (18), the corresponding series approximation for

$$p_1 l_1(t) = \lim_{k \to \infty} \frac{t^2}{2} \sum_{n=0}^k \frac{(-t)^n}{\binom{n+2}{2}} =: \text{pll1ser}(t, k), \text{ where } t = \frac{x - M}{M}.$$
 (23)

This Taylor series expansion is useful and nice, but may not even be needed typically, as both utility functions $\log 1 \text{pmx}(t)$ and $\log 1 \text{p}(t)$ are available, implemented to be fully accurate for small t, $t \ll 1$, and (20), indeed, with t = (x - M)/M the evaluation of

$$D_0(x, M) = M \cdot p_1 l_1(t) = M \cdot \left(\log 1 \operatorname{pmx}(t) + t \cdot \log 1 \operatorname{p}(t) \right), \tag{24}$$

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.p111( -1, 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.p111(-1e-4, 1.5e-4, ylim=1e-8*c(-.6, 1), do.leg=FALSE)
```

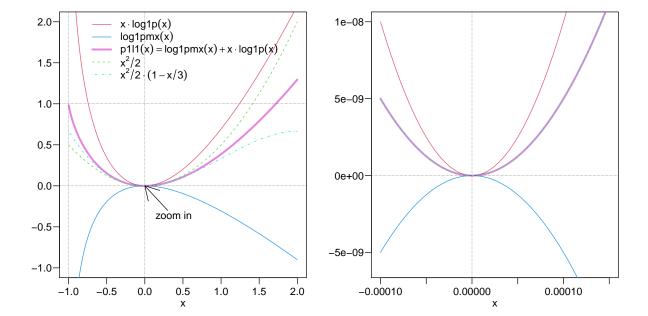


Figure 1: $p_1l_1(t) = p111()$ and its constituents, x*log1p(x) and log1pmx() = log1pmx(), with R functions from our **DPQ** package. On the right, zoomed in 4 and 8 orders of magnitude, where the Taylor approximations $x^2/2$ and $x^2/2 - x^3/6$ are visually already perfect.

Note that $x * \log 1p(x)$ and $\log 1pmx()$ have different signs, but also note that for small |x|, are well approximated by x^2 and $-x^2/2$, so their sum $p_1l_1(x) = \log 1pmx(x) + x \cdot \log 1p(x)$ is approximately $x^2/2$ and numerically computing $x^2 - x^2/2$ should only lose 1 or 2 bits of precision.

Note that in Appendix A.1, we show how using different versions of bd0() computations for computing Poisson density values, dpois(), i.e., our **DPQ** package's dpois_raw() leads to differing accurate results.

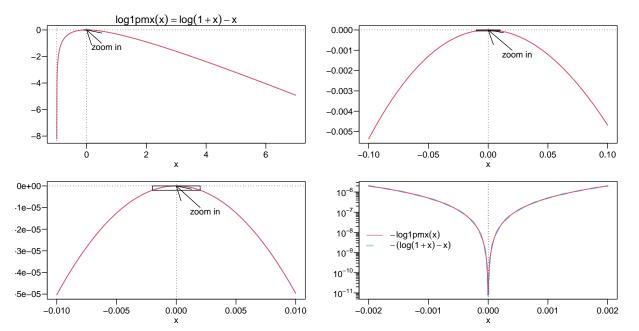
A Accuracy of log1pmx(x) Computations

As we've seen, the "binomial deviance" function $D_0(x, M) = bdO(x, M)$ 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 (24), i.e., with t = (x - M)/M, to compute the sum of two terms $D_0(x, M) = M \cdot (\log 1 \text{pmx}(t) + t \cdot \log 1 \text{p}(t))$.

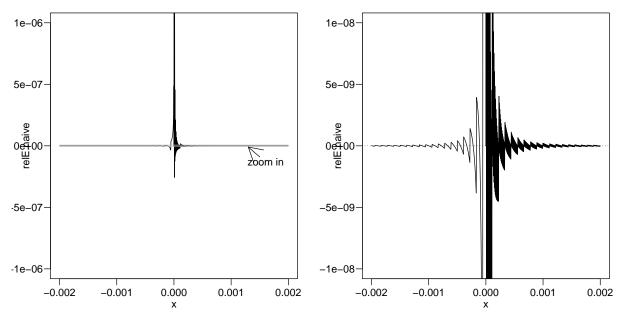
Here, we look more closely at the computation of $\log 1 \text{pmx}(x) := \log(1+x) - x$, at first visualizing the function, notably around (0,0) where numeric cancellations happen if no special care is taken.

```
> lcurve <- function(Fn, a,b, ylab = "", lwd = 1.5, ...)</pre>
      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); zoomToO(1/2, 1)
> lcurve(log1pmx, -.1, .1); rect(-.01, log1pmx(-.01), .01, 0); zoomToO(.02, .001)
> lcurve(log1pmx, -.01, .01); rect(-.002,log1pmx(-.002), .002, 0); zoomToO(2e-3,1e-5)
> lcurve(function(x) -log1pmx(x), -.002, .002, log="y", yaxt="n") -> 11r
> sfsmisc::eaxis(2); abline(v=0, lty=3)
> d1r <- cbind(as.data.frame(l1r), y.naive = with(l1r, -(log(1+x)-x)))
> ## --> d1r is data frame w/ ("x", "y", "y.naive")
> 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")
```



Even if you can't see it in the above 4th plot, 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 of a 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 R to 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?? "../tests/dnbinom-tst.R" rather suggests eps2 = .00163 as optimal for default to1 = 1e-14.))

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

Testing the Poisson probabilities ('density') with several versions of bd0(), ebd0() and ..., we found that using Welinder's proposed ebd0() was advantageous indeed to get full accuracy, and indeed better than all versions of bd0() computations we made available in package **DPQ**. However, the direct formula was more appropriate than ebd0() and all bd0() version for the cases where x/M or M/x were extremely small. Note: Since March 2022 MM has had another (private, uncommitted) tweak in 'src/nmath/dpois.c' to NOT^* use ebd0() nor bd0() but a direct formula, when $2^{-1022} < \frac{x}{\lambda} \le 2^{-52}$, i.e.,

Look at examples in file "../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 $bd0(x,M) := D_0(x,M) := M \cdot p_1 l_1((x-M)/M)$ where we look into providing numerically stable formula for $p_1 l_1(t)$, our p111(t), as its mathematical formula $p_1 l_1(t) = (t+1) \log(1+t) - t$ suffers from cancellation for small |t| even when log1p(t)

is used instead of log(1+t); see the derivations (18), (19), and (21) above, and the Taylor series expansion (22) which we provide in our R functions p111, and p111ser, respectively.

Using a hybrid implementation, p111() uses a direct formula, now the stable one in p111p(), for |t| > c and a series approximation for $|t| \le c$ 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 ?p111, or even run example(p111).

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

Note that the "Stirling error", $\delta(x) \equiv \mathtt{stirlerr}(\mathtt{x})$, $\delta(x) := \log x! - \frac{1}{2} \log(2\pi x) - x \log(x) + x$ 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 (9). A C code implementation had been provided by Loader and for years in R's Mathlib, fur-

A C code implementation had been provided by Loader and for years in R's Mathlib, further improved by the author. Current version in the R sources 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.

Consequently, I have have committed the results to the R sources, svn rev 86191, in March 2024, to be used from R version 4.4.0 on.

References

Loader, C. (2000). Fast and accurate computation of binomial probabilities. Technical report, Lucent; Murray Hill, NJ USA; available at https://www.r-project.org/doc/reports/CLoader-dbinom-2002.pdf.

Welinder, M. (2004). Bug 7307 - pgamma discontinuity. R's PR#7307, comment #6.