Asymptotic Tail Formulas For Gaussian Quantiles

Martin Mächler

Seminar für Statistik, ETH Zurich Nov. 2022 LATEX'ed September 6, 2023

Abstract

R's Gaussian quantile function $\mathtt{qnorm}(\mathtt{p}, \ldots)$ has been based on the published algorithm AS 241 of Wichura (1988) which is fully accurate only on the regular scale for p down to the smallest double precision numbers > 0. When probabilities are used on the log scale, i.e., $\mathtt{qnorm}(\mathtt{lp}, \mathtt{log.p=TRUE})$, the argument is a log probability, and $\mathtt{lp} = \log p \to -\infty$ when $p \to 0$, $\mathtt{qnorm}()$ using AS 241 has been very inaccurate in the very extreme tails.

I have derived novel asymptotic formulas for that case, using recursive plug-in to the asymptotic formula for $\Phi(x)$ (which qnorm() should invert).

Using these formulas for order $k=0,1,\ldots,5$, for six different regions (adjacent intervals) allows to provide fully accurate qnorm() computations also on the log scale. Pure R implementations of these are provided in R package \mathbf{DPQ} (Maechler 2022a), functions qnormAsymp() and qnormR() and have also been prepared to be added to (the C code in Rmathlib in) the next version of R's qnorm().

Keywords: asymptotic, approximation, extreme tail, Gaussian, Normal Quantile, R.

1. Gaussian quantiles in R - okay on regular probability range

Gaussian or normal quantiles have been made available in R (R Core Team 2022), from the very beginning. Ross Ihaka (one of the two "fathers" of R) wrote the first version; visible in R's subversion (svn) repository, rev 574, dated Jan. 14, 1998 basically interfacing R with a C version of the published AS 111 algorithm (which was in Fortran 66 with GOTO etc), Beasley and Springer (1977), but improving AS 111 already by using a more accurate formula from Wichura for the "outer" tail (defined to have $p':=\min(p,1-p)$ close to zero, specifically, when $p' \in (10^{-300},\epsilon_c]$, where ϵ_c , the computer epsilon, (= DBL_EPSILON in C's math library = R's .Machine\$double.eps is nowadays always $\epsilon_c = 2^{-52} = 2.220446..\cdot 10^{-16}$.

This first algorithm AS 111, e.g., in R 1.0.0, Feb.29, 2000, (svn rev 7639, 2000-01-18), the version of <R>/src/nmath/qnorm.c had contained the description

Compute the quantile function for the normal distribution.

For small to moderate probabilities, algorithm referenced below is used to obtain an initial approximation which is polished with a final Newton step.

For very large arguments, an algorithm of Wichura is used.

and the reference to Beasley and Springer (1977).

Also, already before releasing R 1.0.0 on Feb. 29, 2000, as R Core team, we had introduced the log.p and lower.tail logical switches,

```
 r7615 \mid maechler \mid 2000-01-17 \; 12:18:30 \; +0100 \; (Mo, 17 \; Jan \; 2000) \\ add \; new \; argument \; lower.tail \; and \; log[p]; \; at \; first \; only \; to \; [dpq]pois() \\ r7639 \mid maechler \mid 2000-01-18 \; 12:10:44 \; +0100 \; (Di, 18 \; Jan \; 2000) \\ [dpq]norm() \; \& \; [dpq]lnorm() \; have \; new \; args \\
```

Already a few months after releasing R 1.0.0 (June 6, svn r9464), I had switched qnorm() to use the more recent and accurate AS 241 with NEWS entry

o qnorm() is now based on AS 241 instead of AS 111, and should give precise results up to 16 digits precision.

Algorithm AS 241 is by Wichura (1988) which contains the promise of 16 digits precision¹, the last sentence on p.477: ... for $10^{-316} < \min(p, 1-p)$. The second routine, PPND16, is accurate to about 16 figures over the same range.

Also in Wichura (1988),

$$r := \sqrt{-\log(\min(p, 1 - p))} \ (\iff \min(p, 1 - p) = e^{-r^2}).$$
 (1)

For ease of notation, we assume $p < \frac{1}{2}$, for now, and hence the quantile $\operatorname{qnorm}(p) = \Phi^{-1}(p) = \Phi^{-1}(\exp(-r^2))$ is negative. The "outermost" minimax rational approximation to $-\Phi^{-1}(p)$ used in AS 241 is in the interval $r \in (5, 27] \iff r^2 \in (25, 729]$, or equivalently,

$$p \in [e^{-729}, e^{-25}) \approx [2.51 \cdot 10^{-317}, 1.389 \cdot 10^{-11}).$$
 (2)

At first, the above seems sufficient, since indeed, the lower bound is already "de-normalized" in double precision, $e^{-27^2}=e^{-729}\approx 2.51\cdot 10^{-317}$ is smaller than DBL_XMIN in C's math library = R's .Machine\$double.xmin= $2^{-1022}\approx 2.225\cdot 10^{-308}$.

However, as mentioned above, in the R core team we had already seen that it is often advisable to work on the log-scale with probabilities and therefore had introduced the option log.p = TRUE for all our (cumulative) distribution and quantile functions. Now this changes the picture of "sufficient" approximation dramatically, as, indeed, on the log scale, the AS 241 algorithm only goes up to $log p = r^2 = 729$, and then quickly loses precision (see below).

The goal of the remaining part of this paper is to describe the research for finding accurate approximations in these outermost tails.

1.1. DPQ's qnormR() - documenting R history

Note that in \mathbf{DPQ} , pure R code implementations of R's qnorm() are provided by function qnormR() which has (almost²) the same arguments p, mu = 0, sd = 1, lower.tail = TRUE, log.p = FALSE as R's qnorm() and additionally trace = 0, version = c("4.0.x", "2020-10-17", "2022-08-04"), where the default version = "4.0.x" corresponds to R version up to 4.0.5 (2021-03-31) which uses basically the above AS 241, additionally treating extreme cases including $\pm Inf$ and NA, NaN well.

¹16 digits precision, i.e., about the usual IEEE 52-bit double precision ($\epsilon_c = 2^{-52} \approx 2.22 \cdot 10^{-16}$)

 $^{^{2}}$ 'mu' \neq 'mean'

These versions are explained subsequently, starting with the "4.0.x" version which may be considered as "catastrophically wrong" if we look closely in log scale:

2. Correcting qnorm(.., log.p=TRUE)

In order to compare versions of qnorm() approximations with their "true" values, we use the fact that it, $x = \Phi^{-1}(p) = \text{qnorm}(p)$, is defined as *inverse* of $p = \Phi(x) = \text{pnorm}(x)$ and we additionally assume that pnorm(x) is "fully accurate" which it basically is, also on the log scale, demonstrably, e.g., using CRAN pkg **Rmpfr** (Maechler 2022b), with its own very accurate pnorm()³, but we are not providing the evidence here.

With this assumption, the error of qnorm() is the deviation from the identity $\Phi^{-1}(\Phi(x)) \equiv x$. If $x \neq 0$, the relative error is

$$\frac{\widehat{\Phi^{-1}}(\Phi(x)) - x}{x} = \widehat{\Phi^{-1}}(\Phi(x))/x - 1, \tag{3}$$

and we "define" the relative error of qnorm() as qnorm(pnorm(x)) / x - 1 where we need to adjust for cases where x is (very close to) zero or not finite, etc. This is done by function relErrV() from package sfsmisc (Maechler 2022c), shown in the appendix A, which takes care of all special or boundary cases.

And as a matter of fact, we will work in log scale, hence using log.p = TRUE in both pnorm() and qnorm(), and we want to use positive numbers both for argument and result (and nicer formulae), so work with the *upper tail*, i.e., use lower.tail = FALSE. Consequently, instead of computing and inverting $\Phi(x)$, i.e., our qnorm(.) should compute the inverse of $\log(1 - \Phi(x))$.

```
> qs <- 2^seq( 0, 29, by=1/256) # => s >= 1.84
> lp <- pnorm(qs, lower.tail=FALSE, log.p=TRUE)</pre>
> s < -1p \# = -pnorm(...) = -log(1 - Phi(qs)) > 0
> require("DPQ") # --> qnormR():
         <- qnorm (-s, lower.tail=FALSE, log.p=TRUE)
> qnrm405 <- qnormR(-s, lower.tail=FALSE, log.p=TRUE, version= "4.0.x") # R <= 4.0.5
> qnrm410 <- qnormR(-s, lower.tail=FALSE, log.p=TRUE, version= "2020-10-17")
> qnrm43 <- qnormR(-s, lower.tail=FALSE, log.p=TRUE, version= "2022")
> Rver <- sfsmisc::shortRversion()</pre>
> if(getRversion() \le "4.0.5")  { # our qnormR(.., version="4.0.x")
       cat(sprintf("%s, \"4.0.5\",\n
                                       all.equal(*, tol=0): %s; identical(): %s\n", Rver,
                   all.equal(qnrm, qnrm405, tolerance=0), identical(qnrm, qnrm405)))
       stopifnot(all.equal(qnrm, qnrm405, tolerance = 1e-12))
   } else if(getRversion() < "4.3") { # our qnormR(*, version="2020-10-17") matches:
       cat(sprintf("%s, \"4.1.0\", \ all.equal(*, tol=0): %s; identical(): %s\", Rver,
                   all.equal(qnrm, qnrm410, tolerance=0), identical(qnrm, qnrm410)))
       stopifnot(all.equal(qnrm, qnrm410, tolerance = 1e-12))
  } else { \# R version >= 4.3.x
                                     all.equal(*, tol=0): %s; identical(): %s\n", Rver,
       cat(sprintf("%s, >= 4.3.x, n)
                   all.equal(qnrm, qnrm43, tolerance=0), identical(qnrm, qnrm43)))
```

³Rmpfr::pnorm(<mpfr>) is limited in range because it currently has no log scale (or otherwise scaled) version, and we need to take explicit log(.) the values it computes from its pnorm(x) := $\operatorname{erfc}(\sqrt{2} \cdot x)/d$) which underflow to zero before x == 1e6 even with extended mpfr erange.

```
rE6 <- qnorm(-1e6, log.p=TRUE)/-1414.2077829910174 - 1
       cat(sprintf(" rE(-1e6) = %g\n", rE6))
        if(abs(rE6) < 7e-16) # have R-devel with new 2022 code:
            stopifnot(all.equal(qnrm, qnrm43, tolerance = 1e-14))
   }
R 4.3.1 Patched 2023-09-05 r85079, >= 4.3.x,
   all.equal(*, tol=0): TRUE; identical(): TRUE
  rE(-1e6) = 0
Computing a version of the above (with larger range for s, qs <- 2^seq(0,70,by=1/8)) in
R version 4.0.5 and plotting in log-log scale,
> plot(qnrm405 ~ s, type="1", log="xy", col=2, ylim = c(1, max(qs)), asp = 1,
         xaxt="n", yaxt="n"); require("sfsmisc"); eaxis(1); eaxis(2)
> lines(qs ~ s, col=(c4 <- adjustcolor(4, 1/4)), 1wd=4)
> legend("top", c("qnorm(-s, lower.tail=FALSE, log.p=TRUE)", "true"),
           col=c(palette()[2], c4), lwd=c(1,4), bty="n")
                                     qnorm(-s, lower.tail=FALSE, log.p=TRUE)
                                     true
                               10^9 \ 10^{12} \ 10^{15} \ 10^{18} \ 10^{21} \ 10^{24} \ 10^{27} \ 10^{30} \ 10^{33} \ 10^{36} \ 10^{39} \ 10^{42}
```

Figure 1: Extreme tail log scale qnorm(-s, ..) in R 4.0.5 or earlier, i.e., up to 2021; note that true is just lines(qs~s, ..)

Figure 1 looks good up to about 10^{12} , i.e., qnorm() coinciding with the true x qs, but beyond 10^{14} diverging for larger s, and for even larger s showing complete loss of accuracy as qnorm(-s, *) converges (to 98340296.6), even though the true function should go to $+\infty$. We will see that indeed, asymptotically, qnorm(|s|,...) $\sim \sqrt{2|s|}$ which in log-log scale is a line (with intercept $\log \sqrt{2}$ and slope 1/2).

Closer inspection, showing the relative errors in Figure 2:

> $relE_qn \leftarrow relErrV(qs, qnrm405)$; $version.txt \leftarrow "R versions up to R 4.0.5"$

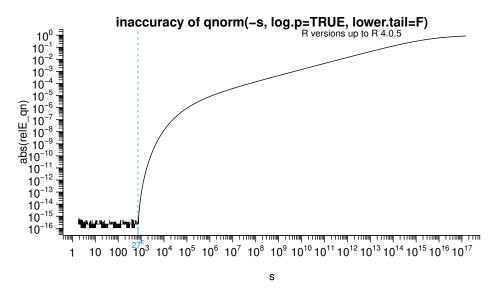


Figure 2: Relative error of qnorm() in extreme tails in R version before R 4.1.0

From this, in September 2020, I started to investigate the visually obvious asymptotic behavior of the *correct* inversion of <code>qnorm()</code>, using the classical first order asymptotic

$$1 - \Phi(x) \sim \frac{\phi(x)}{x}, \quad \text{for } x \to \infty,$$
 (4)

for the standard normal / Gaussian density $\phi(x) := \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ and cumulative distribution function $\Phi(x) := \int_{-\infty}^{x} \phi(t) dt$. On the log scale, this is equivalent to

$$\log(1 - \Phi(x)) = \log \phi(x) - \log x + o(x),$$

$$= -x^2/2 - 1/2 \log 2\pi - \log x + o(x)$$

$$= -x^2/2 + o(x),$$
(5)

as $O(\log x) = o(x)$, i.e., $l_p := \log(1 - \Phi(x)) \approx -x^2/2$ for large x and hence,

$$x \approx \sqrt{-2l_p},\tag{6}$$

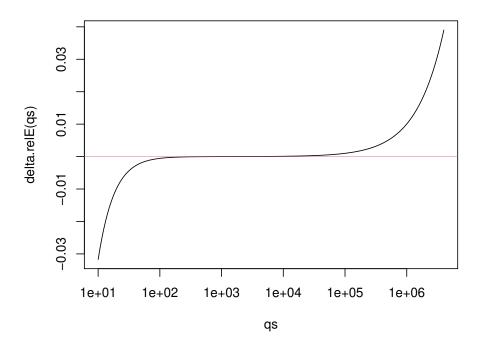
for large |x| or large $|l_p| = -l_p =: s$ (using notation as in the R code above with lp and s <-lp).

Consequently, a first order remedy against the "catastrophic" precision loss for extreme tail qnorm() was to use the above $\sqrt{2s}$ approximation for upper tail probabilities specified in log scale.

Computer experimentation was used to find a numerically optimal (for the double precision implementation of AS 241) cutoff.

Computing the difference ("delta") betwen the absolute value of the relative errors for R 4.0.x's qnorm() and for the asymptotic approximation (6):

```
> delta.relE <- function(q, qNorm = function(...) qnormR(..., version = "4.0.x")) {
    lp <- pnorm(q, lower.tail=FALSE, log.p=TRUE) # <==> q = true qnorm(lp, *)
    ## the "delta" of the two relative errors qnorm() vs sqrt(2*s) approx:
    abs(1 - qNorm(lp, lower.tail=FALSE, log.p=TRUE) / q) -
    abs(1 - sqrt(-2*lp) / q)
    }
> plot(delta.relE(qs) ~ qs, subset = 10 < qs & qs < 4e6, type="1", log="x")
> abline(h=0, col = adjustcolor(2, 1/2))
```



looks like a well

defined zero, we now determine the root location as the optimal cutoff, as it will minimize the absolute value of the relative error of computing qnorm(..). At first:

```
> cutP. <- uniroot(function(logq) delta.relE(exp(logq)) , c(3, 13))
> exp(cutP.$root)
[1] 1153.223
then, getting more accurate once we approximately know the region:
> str(cP. <- uniroot(delta.relE, interval = c(1000, 1300), tol = 1e-12))
List of 5
 $ root
             : num 1153
             : num 0
 $ f.root
             : int 7
 $ iter
 $ init.it
           : int NA
 $ estim.prec: num 2.43e-09
> qC <- cP.$root # 1153.242
> (lpC <- pnorm(qC, lower.tail=FALSE, log.p=TRUE))</pre>
[1] -664991
```

so the optimal cutoff where to use the sqrt-approximation is at $lp = \log p = -664991$ or $r = \sqrt{s} = \sqrt{-\log p} = 815.470$ (with r defined in Equation 1), and for convenience (round number), using the cutoff $r \ge 816$ in qnorm(), i.e., basically

```
if(r \ge 816) value = sqrt(2) * r;
```

This consequently was added to the R (i.e., "R-devel") sources after more testing, a few weeks later

svn r79346 | maechler | 2020-10-17 21:42:17 +0200

to be in R 4.1.0 with NEWS entry

• qnorm(<very large negative>, log.p=TRUE) is now correct to at least five digits where it was catastrophically wrong, previously.

Indeed, qnorm() was now "first order accurate" even in the extreme tails, and in a plot such as Figure 1 one would not notice any inaccuracy. But then, there you'd visually only notice deviations in the order of 1 %, i.e, already visible in 2 digits accuracy. Looking at the relative errors directly in Figure 3 (cf. Figure 2 for the original version), indeed shows that the relative error now is smaller than 10^{-5} and maximal at the cutoff $s = 816^2 = 665856$:

> relE_qn <- relErrV(qs, qnrm410); version.txt <- "R 4.1.0 to 4.2.x"

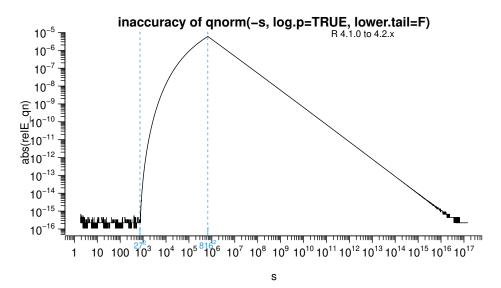


Figure 3: qnorm() relative error in extreme tails, R ver. 4.1.0-4.2.x, ca. 2021-'22

3. Fully accurate asymptotic qnorm(., log.p=TRUE)

In R, the function qnorm() and notably the underlying C API function qnorm()⁴ are used in other places, not the least also to (approximately) compute quantiles of other distributions, such as the (non central) t.

In addition, $\Phi^{-1}(x)$ is a very smooth monotone function, it may naturally be desirable that qnorm() computes its values to the same full (double precision) accuracy as most other mathematically well defined functions in R.

⁴R's C API qnorm() is an alias for qnorm5() in the source file <R>/src/nmath/qnorm.c

Now, the classical simple first order asymptotic (4) for $\Phi(.)$, i.e., R's pnorm(), has been known to many more terms, also for a long time. Mills (1926) builds already on work by Laplace, said to have derived some of the two asymptotic series, in Abramowitz and Stegun (1972)[p. 932],

A. & S. (26.2.12).

$$1 - \Phi(x) = \Phi(-x) = \frac{\phi(x)}{x} \cdot \left(1 - \frac{1}{x^2} + \frac{1 \cdot 3}{x^4} + \dots + \frac{(-1)^n \ 1 \cdot 3 \cdots (2n-1)}{x^{2n}}\right) + R_n, \quad (7)$$

where the remainder term R_n (which can be represented exactly as an integral) is smaller than the first neglected term. Note that A.&S. use notation $Q(x) \equiv 1 - \Phi(x)$ and $Z(x) \equiv \phi(x)$, also in the subsequent asymptotic series which is slightly more accurate numerically (but without an explicit remainder term):

A. & S. (26.2.13).

$$1 - \Phi(x) \sim \frac{\phi(x)}{x} \cdot \left(1 - \frac{a_1}{x^2 + 2} + \frac{a_2}{(x^2 + 2)(x^2 + 4)} - \frac{a_3}{(x^2 + 2)(x^2 + 4)(x^2 + 6)} + \cdots \right), \quad (8)$$
where $a_1 = a_2 = 1, a_3 = 5, a_4 = 9, a_5 = 129,$

and the general coefficient a_n is defined via coefficients of a polynom expansion. As previously, we need to use this in log-scale,

$$l_{p} = \log(1 - \Phi(x)) \approx \log(\phi(x)) - \log(x) + \log(1 - q(x^{2})),$$

$$= -\frac{x^{2}}{2} - \frac{1}{2}\log(2\pi) - \log(x) + \log(1 - q(x^{2})),$$

$$\text{where } q(x^{2}) = \frac{1}{x^{2} + 2} - \frac{1}{(x^{2} + 2)(x^{2} + 4)} + \frac{5}{(x^{2} + 2)(x^{2} + 4)(x^{2} + 6)} + \cdots,$$

$$= \frac{1}{x^{2} + 2} \left(1 - \frac{1}{x^{2} + 4} \left(1 - \frac{1}{x^{2} + 6} \left(5 - \frac{9}{x^{2} + 8} + \cdots\right)\right)\right),$$
(10)

and l_p is the log probability (given as first argument to $\mathtt{qnorm}()$), and we would like to solve for x, as in the simple 1^{st} order case in (5) and (6) above, but of course that is not possible. However, an amazingly versatile idea of recursive "plug-in" will work here: For the first step, we may neglect $q(x^2) \approx 1/(x^2+2)$ entirely as we know that $x^2 \approx 2s$ for relatively large s, and hence drop $\log(1-q(x^2)) \approx \log(1) = 0$, such that $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s, and hence drop $s^2 \approx 2s$ for relatively large s.

$$-2l_p = 2s \approx x^2 + \log(2\pi) + 2\log(x) = x^2 + \log(2\pi x^2), \tag{11}$$

now subtracting the log term and replacing its x^2 by its asymptotic approximation $x_0^2 = 2s$ gives

$$2s - \log(2\pi \ 2s) \approx x^2$$
, or, with
$$x_0^2 := 2s, \tag{12}$$

$$x^{2} \approx x_{1}^{2} := 2s - \log(2\pi \ x_{0}^{2}) = 2s - \log(4\pi s), \tag{13}$$

and we do have a substantially better approximation, verified empirically in Figure 4 below (k = 0 vs k = 1), where we show further steps, continuing to recursively plug in x^2 itself, now no longer neglecting $q(x^2)$ but still only using a first term, from Equation 9,

$$-2\log(1 - \Phi(x)) = 2s \approx x^2 + \log(2\pi \ x^2) - 2\log(1 - q(x^2)) \approx x^2 + \log(2\pi \ x^2) + 2q(x^2), \tag{14}$$

where the 2nd " \approx " is from $\log(1-q)\approx -q$ for $|q|\ll 1$ and $q(x^2)\approx 1/(x^2+2)$ is assumed to be very small here. Again solving for the first x^2 and replacing the other x^2 by our current best approximation x_1^2 leads to

$$x^2 \approx x_2^2 := 2s - \log(2\pi \ x_1^2) - 2/(x_1^2 + 2),$$
 (15)

and continuing recursively, always taking one more term for $q(x^2)$, but no longer replacing $\log(1-q)$ by -q but rather the fully accurate $\log 1p(-q)$,

$$\begin{split} x^2 &\approx x_3^2 := 2s - \log(2\pi \ x_2^2) + 2 \log \ln(-(1 - 1/(4 + x_2^2))/(2 + x_2^2)), \quad \text{and} \quad x^2 \approx \\ x_4^2 &:= 2s - \log(2\pi \ x_3^2) + 2 \log \ln(-(1 - (1 - 5/(6 + x_3^2))/(4 + x_3^2))/(2 + x_3^2)), \quad \text{and} \quad (17) \\ x_5^2 &:= 2s - \log(2\pi \ x_4^2) + 2 \log \ln(-(1 - (1 - (5 - 9/(8 + x_4^2))/(6 + x_4^2))/(4 + x_4^2))/(2 + x_4^2)) \end{split}$$

Taking the square roots of these 6 approximations for x^2 for the inverse cumulative normal, $\Phi^{-1}(e^{-s})$, namely

$$x_0(s) = \sqrt{2s}$$
, from (12)
 $x_1(s) = \sqrt{2s - \log(4\pi s)}$, from (13)
 $x_2(s) = \sqrt{2s - \log(2\pi x_1^2) - 2/(x_1^2 + 2)}$, from (15)
 $x_3(s) = \sqrt{2s - \log(2\pi x_2^2) + 2\log(x_2^2)}$, see (16)
 $x_4(s) = \dots, x_5(s) = \dots$, see (17), (18),

these $x_k(s)$ are provided as plain R function qnormAsymp(), in our **DPQ** package, specifically, $x_k(s) = \text{qnormAsymp(lp = -s, order = k)}^5$

- > k.s <- 0:5; nks <- paste0("k=", k.s)
- > qnAsym <- sapply(setNames(k.s, nks), function(k) qnormAsymp(lp=lp, order = k))
- > relEasym <- apply(qnAsym, 2, relErrV, target = qs) # rel.errors for all

In Figure 4 we depict the absolute values of their respective relative errors (in log-log scale against $s = -lp = -\log(1 - \Phi(x))$), and and then zoom in more closely in Figure 5:

 $^{^5}$ which is the short form; indeed, qnormAsymp(lp = lp, order = k) is identical to qnormAsymp(p = lp, lower.tail=FALSE, log.p=TRUE, order = k).

```
> matplot(-lp, abs(relEasym), log="xy", type="l", lwd=2, axes=FALSE, xlab = quote(s == -lp))
> eaxis(1, sub10=2); eaxis(2, sub10=c(-2,2), nintLog=16); grid(col="gray75")
> legend("right", nks, col=1:6, lty=1:5, lwd=2, bty="n")
             0.1
            0.01
            10<sup>-3</sup>
            10^{-4}
            10^{-5}
        k=0
                                                                                                                   k=1.
                                                                                                                   k=3
                                                                                                                   k=4
                                                                                                                   k=5
           10^{-11}
           10<sup>-12</sup>
           10<sup>-13</sup>
           10<sup>-14</sup>
           10<sup>-15</sup>
           10<sup>-16</sup>
                             citing riting ritin
                               100 \ 10^{3} \ 10^{4} \ 10^{5} \ 10^{6} \ 10^{7} \ 10^{8} \ 10^{9} \ 10^{10} \ 10^{11} \ 10^{12} \ 10^{13} \ 10^{14} \ 10^{15} \ 10^{16} \ 10^{17}
```

s = -lp

Figure 4: |relative errors| of asymptotic approximations in log-log scale

Martin Mächler

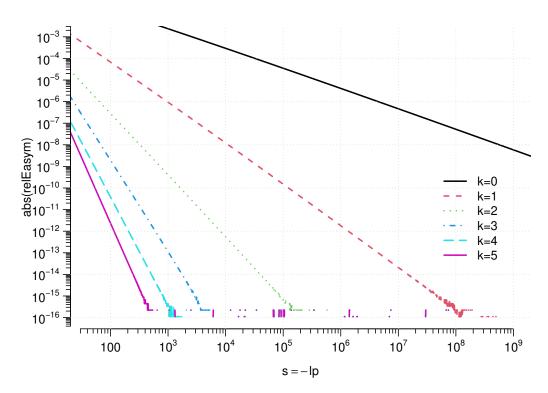


Figure 5: (Zoomed Fig. 4) | relative errors | of asymptotic approx. $x_0(s), x_1(s), \ldots, x_5(s)$

Fully accurate qnorm()

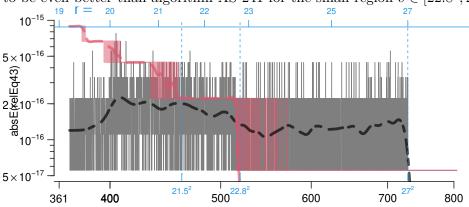
Our package **DPQ**'s qnormR(... version = "2022-08") now implements a (pure R implementation) also to be used (in C) in the next version of R, which uses "the optimal" asymptotic approximation $x_k(s)$ for $s = r^2 > 27^2$ and $k \in \{0, 1, ..., 5\}$ as defined above in (12)-(18). "Optimal" is defined as the smallest k which still provides full accuracy, e.g., when $s > 10^{18}$ clearly, $x_0(s) = \sqrt{2s}$ is sufficient and hence optimal in that sense.

Consequently, we have determined ("round number", approximate) **optimal cut points** / **regions for different approximation orders** k and found the following "round number" values,

k	5	4	3	2	1	0
$r \ge$	1				0000	6.4e8
$s = r^2 \ge$	729	3025	11880	705600	$1296 \cdot 10^6$	4.096e17

Table 1: Optimal cutpoints to determine k to use $x_k(s)$ for $r = \sqrt{s} > 27$.

e.g., k=0 is fully accurate and hence optimal and used for $r \geq 6.4e8 = 640 \cdot 10^6$, or equivalently, for $s=-\text{lp} \geq 4.096e17$, where as for $r \in [55,109) \iff s \in [3025,11880)$ one needs (and uses) k=4. These were determined using function p.qnormAsy2() in appendix B, for visualizing the optimal region for switching from k-1 to k, for k=1,2,3,4,5, see Figure 6. Empirically, we see that now most relative errors are numerically zero and the others are at most $\epsilon_c = 2^{-52} \approx 2.22 \cdot 10^{-16}$, indeed the asymptotic $x_5(s)$, see Equation 18, may be seen



to be even better than algorithm AS 241 for the small region $s \in [22.8^2, 27^2] = [519.84, 729]$.

> relE_qn <- relErrV(qs, qnrm43)</pre>

We tabulate the values as multiples of ϵ_c not needing a visualization:

```
> table(2^52 * relE_qn)
                                    # all in [-2.5, 3]
                                        2
-2.5
       -2 - 1.5
                  -1 -0.5
                                              3
            97
                282 356 6264
                                 370
                                       21
                                              1
> table(2^52 * relE_qn[s > 27^2]) #
                                           in [-1,
                                                     1]
  -1 -0.5
             0
  36
     129 5763
                152
```

To see how the final qnormR() is implemented, you can look at the length-1 version qnormR1()⁶.

4. Concluding summary

We have derived novel asymptotic formulas for qnorm(1p, lower.tail=FALSE, log.p=TRUE), i.e., $\Phi^{-1}(e^s) = \Phi^{-1}(e^{r^2})$ for large $s=r^2$, notably for r>27 which is beyond the range where the published algorithm AS 241, Wichura (1988), is accurate, see (12), (13), and (15)–(18). For these formulas of order $k=0,1,\ldots,5$, implemented in **DPQ**'s R function qnormAsymp(*, order=k) we have derived optimal regions, i.e., intervals for r, partitioning $(27,\infty)$, see Table 1, and implemented in R function qnormR(*, version = "2022-08") for reproducibility and to be used in (the C code in Rmathlib in) the next version of R's qnorm().

5. Computational details, session information

For most of our plots we made use of utilities for log scale axis drawing, notably eaxis() and also mult.fig() (for p.qnormAsy2() in appendix B) from our package sfsmisc (Maechler 2022c), from which also relErrV() was used, for computing relEasym, plotted in Figure 4 and 5.

- > toLatex(sessionInfo(), locale=FALSE)
 - R version 4.3.1 Patched (2023-09-05 r85079), x86_64-pc-linux-gnu

⁶indeed, in the package source file DPQ/R/norm_f.R, qnormR() is defined to correctly vectorize in its main arguments p, mu, and sd, by qnormR <- Vectorize(qnormR1, c("p", "mu", "sd"))

Martin Mächler 13

- Running under: Fedora Linux 36 (Thirty Six)
- Matrix products: default
- BLAS: /u/maechler/R/D/r-patched/F36-64-inst/lib/libRblas.so
- LAPACK: /usr/lib64/liblapack.so.3.10.1
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: DPQ 0.5-6, sfsmisc 1.1-16
- Loaded via a namespace (and not attached): compiler 4.3.1, tools 4.3.1

A. Function relErrV() (package sfsmisc)

To compute relative (approximation) errors, in a way that works correctly, also with Inf, NA, and NaNs, we make use of the function relErrV() from (our own) CRAN package sfsmisc, defined⁷ as

```
> ## Componentwise aka "Vectorized" relative error:
> ## Must not be NA/NaN unless one of the components is ==> deal with {0, Inf, NA}
> relErrV <- function(target, current, eps0 = .Machine$double.xmin) {</pre>
       n <- length(target <- as.vector(target))</pre>
       ## assert( <length current> is multiple of <length target>) :
       lc <- length(current)</pre>
       if(!n) {
           if(!lc) return(numeric()) # everything length 0
           else stop("length(target) == 0 differing from length(current)")
       } else if(!lc)
           stop("length(current) == 0 differing from length(target)")
       ## else n, 1c > 0
       if(lc %% n)
           stop("length(current) must be a multiple of length(target)")
       recycle <- (lc != n) # explicitly recycle
       R <- if(recycle)</pre>
                 target[rep(seq_len(n), length.out=lc)]
                 target # (possibly "mpfr")
       R[] \leftarrow 0
       ## use *absolute* error when target is zero {and deal with NAs}:
       t0 <- abs(target) < eps0 & !(na.t <- is.na(target))</pre>
       R[t0] <- current[t0]</pre>
       ## absolute error also when it is infinite, as (-Inf, Inf) would give NaN:
       dInf <- is.infinite(E <- current - target)</pre>
       R[dInf] \leftarrow E[dInf]
       useRE <- !dInf & !t0 & (na.t | is.na(current) | (current != target))</pre>
```

 $^{^7} currently; for updates, see \verb|https://github.com/mmaechler/sfsmisc/blob/master/R/relErr.R|$

}

```
R[useRE] <- (current/target)[useRE] - 1
## preserve {dim, dimnames, names} from 'current' :
if(!is.null(d <- dim(current)))
    array(R, dim=d, dimnames=dimnames(current))
else if(!is.null(nm <- names(current)) && is.null(names(R))) # not needed for mpfr
    `names<-`(R, nm)
else R</pre>
```

B. Function p.qnormAsy2() for showing optimal cutpoints

```
This function, currently also used in DPQ's example(qnormAsymp), was used by the author
and may be used for reproducibility to visualize the five "cutpoint - regions", Table 1, to
switch from approximation x_{k-1}(r) to x_k(r), for k=1,\ldots,5 and r=\sqrt{s}=\sqrt{-\log p}, using
> r0 <- c(27, 55, 109, 840, 36000, 6.4e8) # <-- cutoffs <--> in ../R/norm_f.R
                                        0 e.g. k = 0 good for r >= 6.4e8
>  # use k = 5
                          2
                                  1
> for(ir in 2:length(r0)) {
     p.qnormAsy2(r0[ir], k = 5 + 2-ir) # k = 5, 4, ...
     if(interactive() && ir < length(r0)) {</pre>
          cat("[Enter] to continue: "); cat(readLines(stdin(), n=1), "\n") }
   }
> ## Zoom into each each cut-point region :
> p.qnormAsy2 <- function(r0, k, # use k-1 and k in region around r0
                           n = 2048, verbose=TRUE, ylim = c(-1,1) * 2.5e-16,
                           rr = seq(r0 * 0.5, r0 * 1.25, length = n), ...)
   {
     stopifnot(is.numeric(rr), !is.unsorted(rr), # the initial 'r'
               length(k) == 1L, is.numeric(k), k == as.integer(k), k >= 1)
     k.s \leftarrow (k-1L):k; nks \leftarrow paste0("k=", k.s)
     if(missing(r0)) r0 <- quantile(rr, 2/3)# allow specifying rr instead of r0
     if(verbose) cat("Around r0 =", r0,"; k = ", deparse(k.s), "\n")
     1p \leftarrow (-rr^2) \# = -r^2 = -s \iff rr = sqrt(-1p)
     q. <- qnormR(lp, lower.tail=FALSE, log.p=TRUE, version="2022-08")# *not* depending on R ver!
    pq <- pnorm (q., lower.tail=FALSE, log.p=TRUE) # ~= lp
     ## the arg of pnorm() is the true qnorm(pq, ...) == q. by construction
     r <- sqrt(- pq)
     stopifnot(all.equal(rr, r, tol=1e-15))
     qnAsy <- sapply(setNames(k.s, nks), function(ord)</pre>
                     qnormAsymp(pq, lower.tail=FALSE, log.p=TRUE, order=ord))
     relE \leftarrow qnAsy / q. - 1
     m <- cbind(r, pq, relE)</pre>
     if(verbose) {
       print(tail(m, 4))
     ## matplot(r, relE, type = "b", main = paste("around r0 = ", r0))
     matplot(r, relE, type = "l", ylim = ylim,
        main = paste("Relative error of qnormAsymp(*, k) around r0 = ", r0,
                     "for k = ", departs (k.s)),
        xlab = quote(r == sqrt(-log(p))), ...)
```

legend("topleft", nks, horiz = TRUE, col=1:2, lty=1:2, bty="n", lwd=2)

```
for(j \ in \ seq\_along(k.s)) \\ lines(smooth.spline(r, relE[,j]), col=adjustcolor(j, 2/3), lwd=4, lty="6132") \\ cc <- "blue2"; lab <- substitute(r[0] == R, list(R = r0)) \\ abline(v = r0, lty=2, lwd=2, col=cc) \\ axis(3, at= r0, labels=lab, col=cc, col.axis=cc, line=-1) \\ abline(h = (-1:1)*.Machine$double.eps, lty=c(3,1,3), \\ col=c("green3", "gray", "tan2")) \\ invisible(cbind(r = r, qn = q., relE)) \\ \}
```

qnormAsymp(*, k) approximations in the 5 cutpoint regions

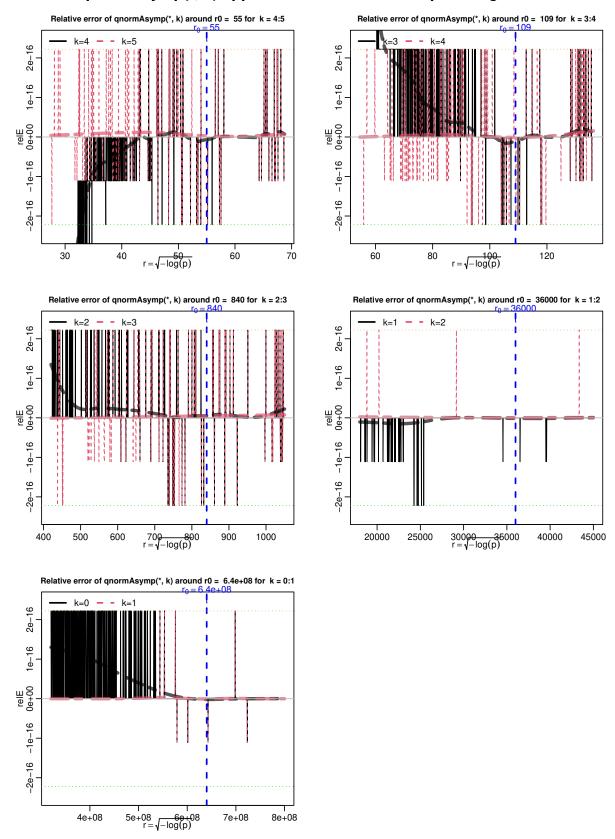


Figure 6: qnormAsymp(*, k) approximation in the 5 cutpoint regions: $r0 \leftarrow c(27, 55, 109, 840, 36000, 6.4e8)$ for(ir in 2:length(r0)) p.qnormAsy2(r0[ir], k = 5 + 2-ir, ...)

References

- Abramowitz M, Stegun IA (1972). *Handbook of Mathematical Functions*. Dover Publications, N. Y. URL https://en.wikipedia.org/wiki/Abramowitz_and_Stegun.
- Beasley JD, Springer SG (1977). "Algorithm AS 111: The Percentage Points of the Normal Distribution." Applied Statistics Journal of the Royal Statistical Society C, 26(1), 118–121. doi:10.2307/2346889.
- Maechler M (2022a). **DPQ**: Density, Probability, Quantile ('DPQ') Computations. R package version 0.5-3, URL https://CRAN.R-project.org/package=DPQ.
- Maechler M (2022b). Rmpfr: R MPFR Multiple Precision Floating-Point Reliable. R package version 0.9-0 from https://rmpfr.R-forge.R-project.org/, URL https://CRAN.R-project.org/package=Rmpfr.
- Maechler M (2022c). sfsmisc: Utilities from 'Seminar fuer Statistik' ETH Zurich. R package version 1.1-14, URL https://CRAN.R-project.org/package=sfsmisc.
- Mills JP (1926). "Table of the Ratio: Area to Bounding Ordinate, for Any Portion of Normal Curve." *Biometrika*, **18**(3-4), 395–400. ISSN 0006-3444. doi:10.1093/biomet/18.3-4. 395.
- R Core Team (2022). R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria. URL https://www.R-project.org/.
- Wichura MJ (1988). "Algorithm AS 241: The Percentage Points of the Normal Distribution." Applied Statistics Journal of the Royal Statistical Society C, 37(3), 477–484. doi: 10.2307/2347330.

Affiliation:

Martin Mächler Seminar für Statistik, HG G 16 ETH Zurich 8092 Zurich, Switzerland

E-mail: maechler@stat.math.ethz.ch URL: http://stat.ethz.ch/~maechler