

Numerically Stable Frank Copula Functions via Multiprecision: R Package Rmpfr

Martin Mächler

ETH Zurich

May 2011 (L^AT_EX'ed April 11, 2012)

Abstract

The package **copula** Archimedean copulas
The package **Rmpfr**

Keywords: Archimedean copulas, Frank Copula, Multiple Precision, R, MPFR, Rmpfr.

1. The diagonal density of Frank's copula

The “diagonal density” of a copula $C(\cdot)$ is the density of $\max(U_1, U_2, \dots, U_d)$, where $\mathbf{U} = (U_1, U_2, \dots, U_d)^T \sim C$. The (cumulative) distribution function, by definition,

$$F^D(u) := P[\max(U_1, U_2, \dots, U_d) \leq u] = P[U_1 \leq u, U_2 \leq u, \dots, U_d \leq u] = C(u, u, \dots, u), \quad (1)$$

evaluates the copula only on the diagonal and is therefore called “*the diagonal of C*”. Its density $f^D(u) := \frac{d}{du} F^D(u)$, is therefore called the diagonal density of C . For Archimedean copulas, i.e., where

$$C(\mathbf{u}) = C(\mathbf{u}; \psi) = \psi(\psi^{-1}(u_1) + \dots + \psi^{-1}(u_d)), \quad \mathbf{u} \in [0, 1]^d, \quad (2)$$

the diagonal density is

$$\begin{aligned} f^D(u) &= \frac{d}{du} F^D(u) = \frac{d}{du} \psi \left(\sum_{j=1}^d \psi^{-1}(u) \right) = \frac{d}{du} \psi(d \cdot \psi^{-1}(u)) = \\ &= \psi'(d \cdot \psi^{-1}(u)) \cdot d \cdot \frac{d}{du} \psi^{-1}(u) \\ &= d \cdot \psi'(d \cdot \psi^{-1}(u)) \cdot [\psi^{-1}]'(u). \end{aligned} \quad (3)$$

For this reason, the **copula** package's `dDiag()` function for computing the diagonal density $f^D(u)$ makes use of the following

```
> copula::dDiagA
function (u, d, cop, log = FALSE)
{
  stopifnot(is.finite(th <- cop@theta), d >= 2)
  if (any(copAMH$name == c("AMH", "Frank", "Gumbel", "Joe")) &&
      any(i0 <- u == 0)) {
```

```

    if (log)
      u[i0] <- -Inf
    u[!i0] <- dDiagA(u[!i0], d = d, cop = cop, log = log)
    return(u)
  }
  if (log) {
    log(d) + cop@psiDabs(d * cop@psiInv(u, th), th, log = TRUE) +
      cop@psiInvD1abs(u, th, log = TRUE)
  }
  else {
    d * cop@psiDabs(d * cop@psiInv(u, th), th) * cop@psiInvD1abs(u,
      th)
  }
}

```

where the three functions

$$\text{psiDabs}(t, \text{thet}) = |\psi'_\theta(t)|, \quad (4)$$

$$\text{psiInv}(u, \text{thet}) = \psi_\theta^{-1}(u), \text{ and} \quad (5)$$

$$\text{psiInvD1abs}(u, \text{thet}) = |[\psi_\theta^{-1}]'(u)| \quad (6)$$

are all provided by the slots of the corresponding Archimedean copula family.

For the following explorations, we need a definition of `dDiagA` which is more flexible as it does not work with the copula family object but gets the three functions as arguments,

```

> dDiagA <- function(u, th, d, psiInv, psiDabs, psiInvD1abs, log = FALSE) {
  stopifnot(is.finite(th), d > 0, is.function(psiInv),
    is.function(psiDabs), is.function(psiInvD1abs))
  if(log) {
    log(d) + psiDabs(d*psiInv(u,th), th, log = TRUE) +
      psiInvD1abs(u, th, log = TRUE)
  } else {
    d* psiDabs(d*psiInv(u,th), th) * psiInvD1abs(u,th)
  }
}

```

Now, for the Frank copula (see Hofert and Mächler (2011)),

$$\psi_\theta(t) = -\frac{1}{\theta} \log \left(1 - (1 - e^{-\theta})e^{-t} \right), \quad \theta > 0, \quad \text{hence,} \quad (7)$$

$$\psi_\theta^{-1}(u) = -\log \left(\frac{e^{-u\theta} - 1}{e^{-\theta} - 1} \right), \quad \text{and} \quad (8)$$

$$(-1)^k \psi_\theta^{(k)}(t) = |\psi_\theta^{(k)}(t)| = \frac{1}{\theta} \text{Li}_{k-1}((1 - e^{-\theta})e^{-t}), \quad \text{and} \quad (9)$$

$$|[\psi_\theta^{-1}]'(u)| = \theta / (e^{u\theta} - 1), \quad (10)$$

where $\text{Li}_s(z)$ is the *polylogarithm of order s* at z , defined as (analytic continuation of) $\sum_{k=1}^{\infty} \frac{z^k}{k^s}$. When $s = -n$, $n \in \mathbb{N}$, one has

$$\text{Li}_{-n}(z) = \left(z \cdot \frac{\partial}{\partial z} \right)^n \frac{z}{1-z}, \quad (11)$$

and we note that here, only the first derivative is needed, $-\psi_\theta'(t) = |\psi_\theta'(t)|$, and hence only

$$\text{polylog}(z, s = 0) = \text{Li}_0(z) = z/(1 - z). \quad (12)$$

First note that numerically, $e^{-a} - 1$ suffers from cancellation when $0 < a \ll 1$, and the R (and C) function `expm1(-a)` is advisably used instead of `exp(-a) - 1`. For this reason, in **copula**, I had replaced the original `psiInv.0(u, th)` for $\psi_\theta^{-1}(u)$ by `psiInv.1()`, making use of `expm1()`. These and the derivative (9) originally were

```
> psiInv.0 <- function(u,theta) -log( (exp(-theta*u)-1) / (exp(-theta)-1) )
> psiInv.1 <- function(u,theta) -log(expm1(-u*theta) / expm1(-theta))
> psiInvDiabs.1 <- function(u, theta, log = FALSE)
  if(log) log(theta)-log(expm1(u*theta)) else theta/expm1(u*theta)
```

and the general k -th derivative (10), simplified, for $k = 1$ (`degree = 1`),

```
> require("copula")# for polylog()
> psiDabs.1 <- function(t, theta, log=FALSE) {
  p <- -expm1(-theta)
  Li. <- polylog(log(p) - t, s = 0, log=log,
    method="negI-s-Eulerian", is.log.z=TRUE)
  if(log) Li. - log(theta) else Li. / theta
}
```

where we however now assume that the `polylog()` function for `s=0` would basically use the direct formula (12), such that we use

```
> psiDabs.2 <- function(t, theta, log=FALSE) {
  w <- log(-expm1(-theta)) - t
  Li. <- if(log) w - log(-expm1(w)) else -exp(w)/expm1(w)
  if(log) Li. - log(theta) else Li. / theta
}
```

2. Computing the “diagonal MLE”

The most important use of the diagonal density is to compute the “diagonal maximum likelihood estimator”, `dmle`, $\hat{\theta}^D$ which for a sample of observations $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n$, ($\mathbf{u}_i \in [0, 1]^d$) is defined as minimizer of the negative log-likelihood,

$$\hat{\theta}^D = \arg \min_{\theta} -l(\theta; \mathbf{u}_1, \dots, \mathbf{u}_n), \quad \text{where} \quad (13)$$

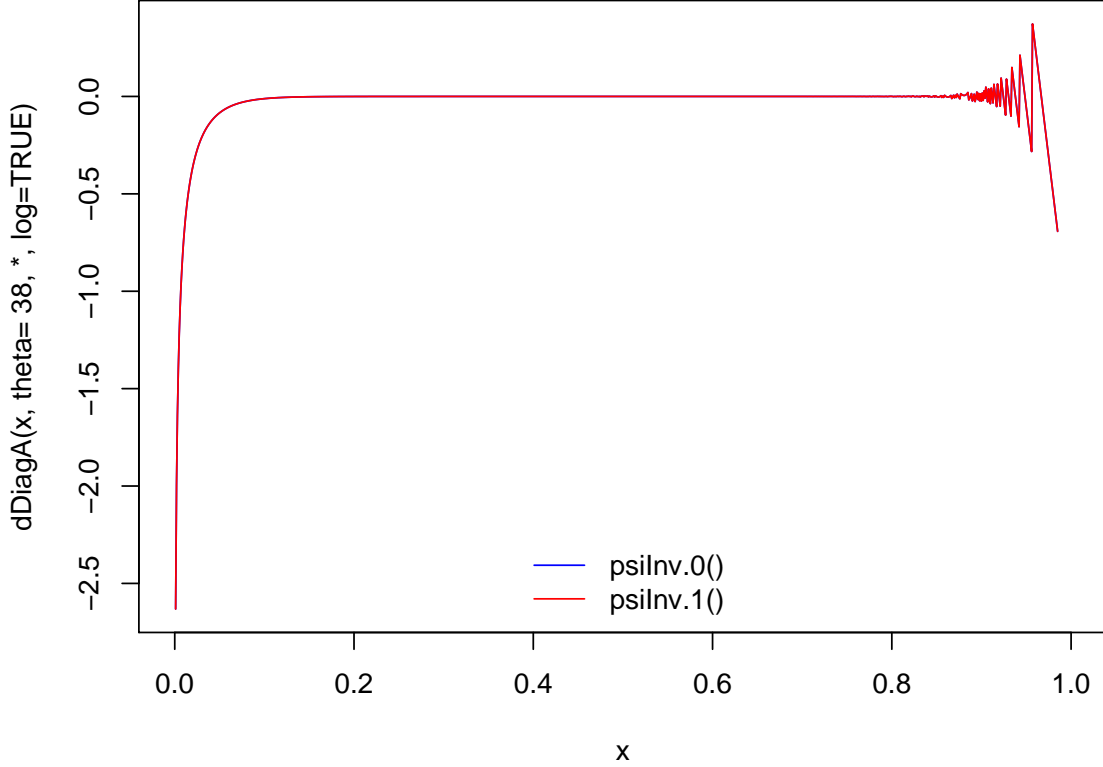
$$l(\theta; \mathbf{u}_1, \dots, \mathbf{u}_n) = \sum_{i=1}^n \log f^D(\tilde{u}_i) \quad \text{and} \quad (14)$$

$$\tilde{u}_i = \max_{j=1, \dots, d} u_{i,j}. \quad (15)$$

In our exploration of the `dmle` estimator, we found cases with numerical problems, at first already in evaluating the logarithm of the diagonal density $\log f^D = \log f_\theta^D(u) = \text{dDiag}(u, \text{theta}, *, \text{log}=\text{TRUE})$ for non-small θ and “large” u , i.e., $u \approx 1$:

```
> curve(dDiagA(x, th = 38, d = 2, psiInv = psiInv.0,
  psiDabs=psiDabs.1, psiInvDiabs=psiInvDiabs.1, log = TRUE),
  ylab = "dDiagA(x, theta= 38, *, log=TRUE)",
  0, 1, col = 4, n = 1000)
```

```
> ## and using the slightly better psiInv.1 does not help here:
> curve(dDiagA(x, th = 38, d = 2, psiInv = psiInv.1,
  psiDabs=psiDabs.2, psiInvD1abs=psiInvD1abs.1, log = TRUE),
  add = TRUE, col = 2, n=1000)
> legend("bottom", c("psiInv.0()", "psiInv.1()"), col=c(4,2), lty=1, bty="n")
```

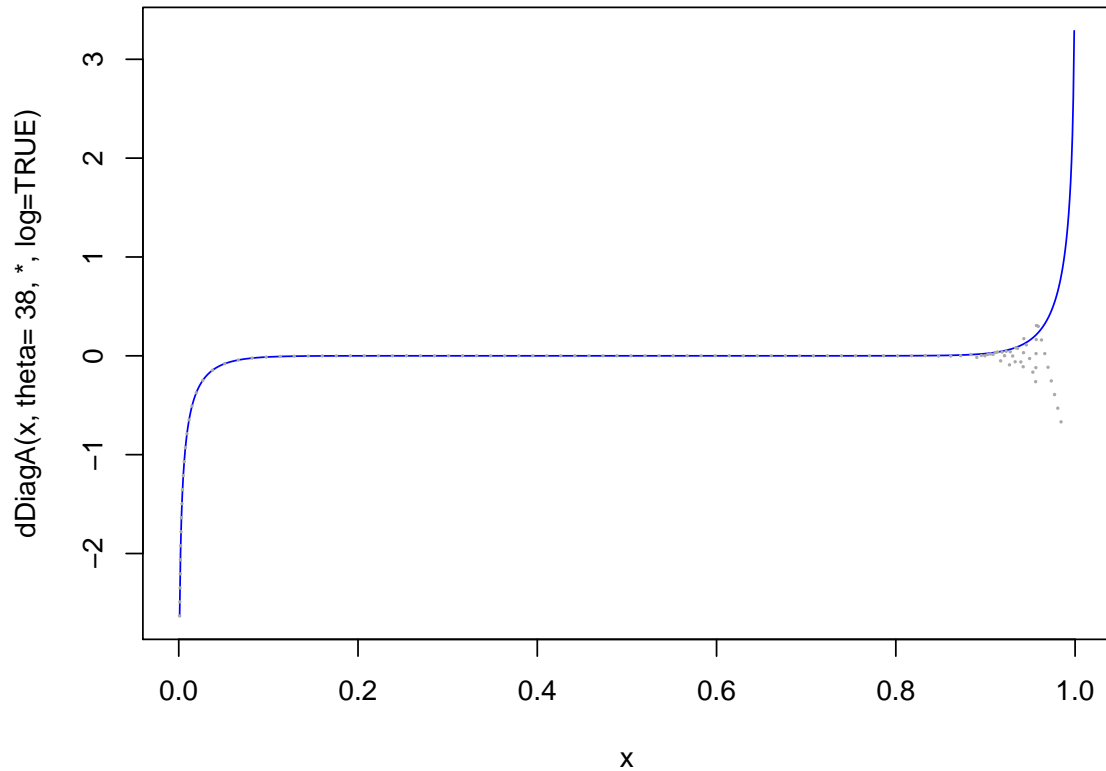


However, it's not hard to see that indeed our initial computation of Frank's ψ^{-1} , i.e, (8), $\psi_{\theta}^{-1}(u) = -\log\left(\frac{1-e^{-u\theta}}{1-e^{-\theta}}\right)$, suffers from "division cancellation" for "large" θ ($\theta = 38$ in ex.) when computed directly with `psiInv.0()`, see above, and that the improvement of using `expm1(-t)` instead of `exp(-t) - 1`, as used in `psiInv.1()`, see above, helps only for $t \approx 0$. However, we can rewrite ψ^{-1} as

$$\psi_{\theta}^{-1}(u) = -\log\left(1 - \frac{e^{-u\theta} - e^{-\theta}}{1 - e^{-\theta}}\right), \quad (16)$$

which when using `log1p(e)` for `log(1 + e)` is much better numerically:

```
> psiInv.2 <- function(u,theta) -log1p((exp(-u*theta)-exp(-theta)) / expm1(-theta))
> curve(dDiagA(x, th = 38, d = 2, psiInv = psiInv.2,
  psiDabs=psiDabs.2, psiInvD1abs=psiInvD1abs.1, log = TRUE),
  ylab = "dDiagA(x, theta= 38, *, log=TRUE)",
  0, 1, col = 4, n = 1000)
> ## previously
> curve(dDiagA(x, th = 38, d = 2, psiInv = psiInv.1,
  psiDabs=psiDabs.2, psiInvD1abs=psiInvD1abs.1, log = TRUE),
  add = TRUE, col = "darkgray", lwd=2, lty=3, n=1000)
```



Unfortunately, this is not enough to get numerically stable evaluations of the negative log-likelihood $l()$:

```
> d <- 5
> (theta <- copFrank@tauInv(tau = 0.75))
[1] 14.1385

> cop <- onacopulaL("Frank", list(theta, 1:d))
> set.seed(1); for(1 in 1:4) U <- rnacopula(n = 100, cop)
> U. <- sort(apply(U, 1, max)) # build the max

> mlogL <- function(theta)
+   -sum(dDiagA(U., theta, d=d, psiInv = psiInv.2,
+             psiDabs=psiDabs.2, psiInvD1abs=psiInvD1abs.1,
+             log = TRUE))
```

Now, plot this negative log likelihood function in an interval θ , close to what is proposed **copula**'s `initOpt()` function, defining a utility function that we'll reuse later:

```
> p.mlogL <- function(th, mlogL, col= "red2", lwd = 1, lty = 1,
+                   add= FALSE) {
+   stopifnot(is.numeric(th), is.function(mlogL))
+   nll <- vapply(th, mlogL, 0.)
+   if(add) lines(nll ~ th, col=col, lwd=lwd, lty=lty)
+   else plot(nll ~ th, xlab=expression(theta),
+             ylab = expression(- logLik(theta, .)),
+             type = "l", col=col, lwd=lwd, lty=lty)
+   invisible(nll) # return invisibly
```

```

}
> thet <- seq(11, 99, by = 1/4)
> p.mlogL(thet, mlogL)
> require("Rmpfr")## compute the same with *high* accuracy ...

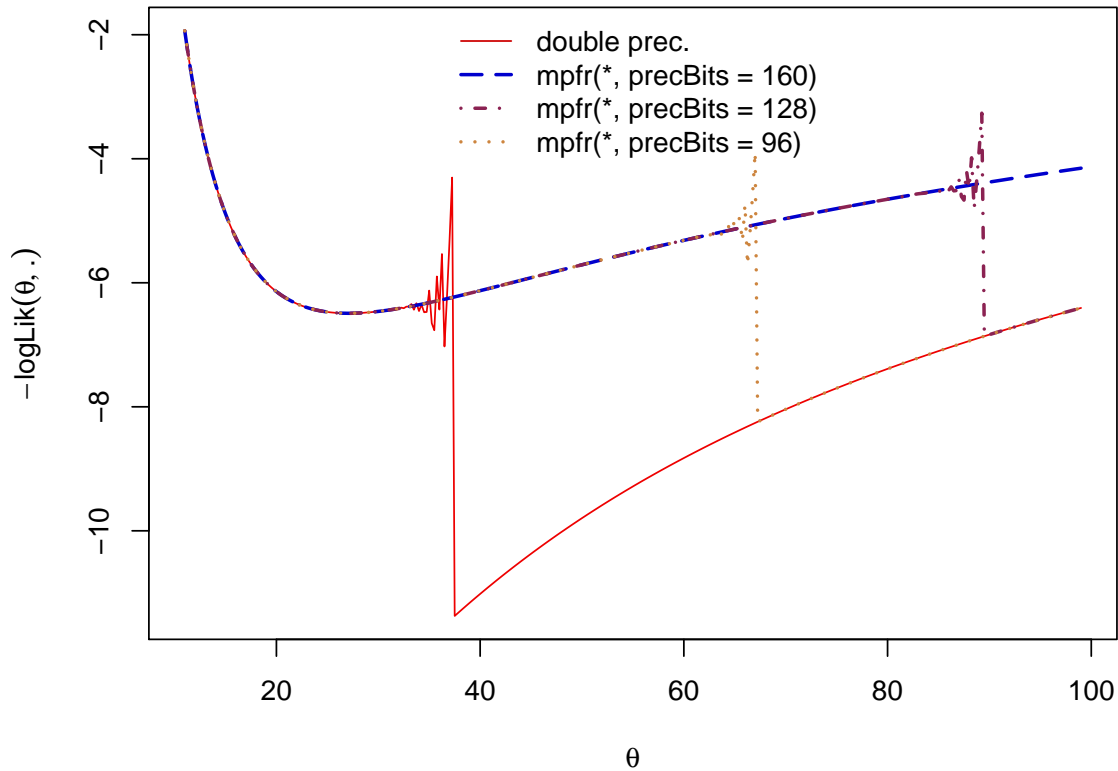
```

Loading C code of R package 'Rmpfr': GMP using 64 bits per limb

```

> ## using three different precisions:
> MPrecBits <- c(160, 128, 96)
> mkNm <- function(bits) sprintf("%03d.bits", bits)
> ## As it takes a while, cache the result:
> fnam <- sprintf("mlogL_mpfr_%s.rda", Sys.info()[["machine"]])
> if (!file.exists(fn <- file.path(copDDir,fnam))) {
  print(system.time(
    nllMP <- lapply(MPrecBits, function(pBit) {
      nLM <- thM <- mpfr(thet, precBits = pBit)
      ## (vapply() does not work for "Rmpfr":)
      for(i in seq_along(thet)) nLM[i] <- mlogL(thM[i])
      nLM
    })
  )) ## 91.226 0.013 91.506 [nb-mm icore 5]
  names(nllMP) <- mkNm(MPrecBits)
  copSrcDDir <- if(Sys.getenv("USER") == "maechler")
    '~/R/Pkgs/copula/inst/doc' else ""
  if(file.exists(copSrcDDir))# <- only for certain users; not on CRAN etc
    save(nllMP, file = file.path(copSrcDDir, fnam))
} else load(fn)
> colB <- c("blue3", "violetred4", "tan3")
> ltyB <- c(5:3)
> lwdB <- c(2,2,2)
> for(i in seq_along(nllMP)) {
  lines(thet, as.numeric(nllMP[[i]]),
        col=colB[i], lty = ltyB[i], lwd = lwdB[i])
}
> leg <- c("double prec.", sprintf("mpfr(*, precBits = %d)", MPrecBits))
> legend("top", leg,
        col= c("red3",colB), lty=c(1, ltyB), lwd=c(1,lwdB), bty="n")

```



So, clearly, high-precision computations can solve the numerical problems, if the precision is high enough. E.g., for $\theta = 100$, it needs more than 128 bits precision.

Let us look at the phenomenon in more details now. The flesh in the `mlogL()` computation is (up to the constant $\log(d)$, $d = 5$), only the sum of the two terms

```
psiDabs(d*psiInv(u,th), th, log = TRUE) +
psiInvDlabs(u,          th, log = TRUE)
```

currently, with the three functions

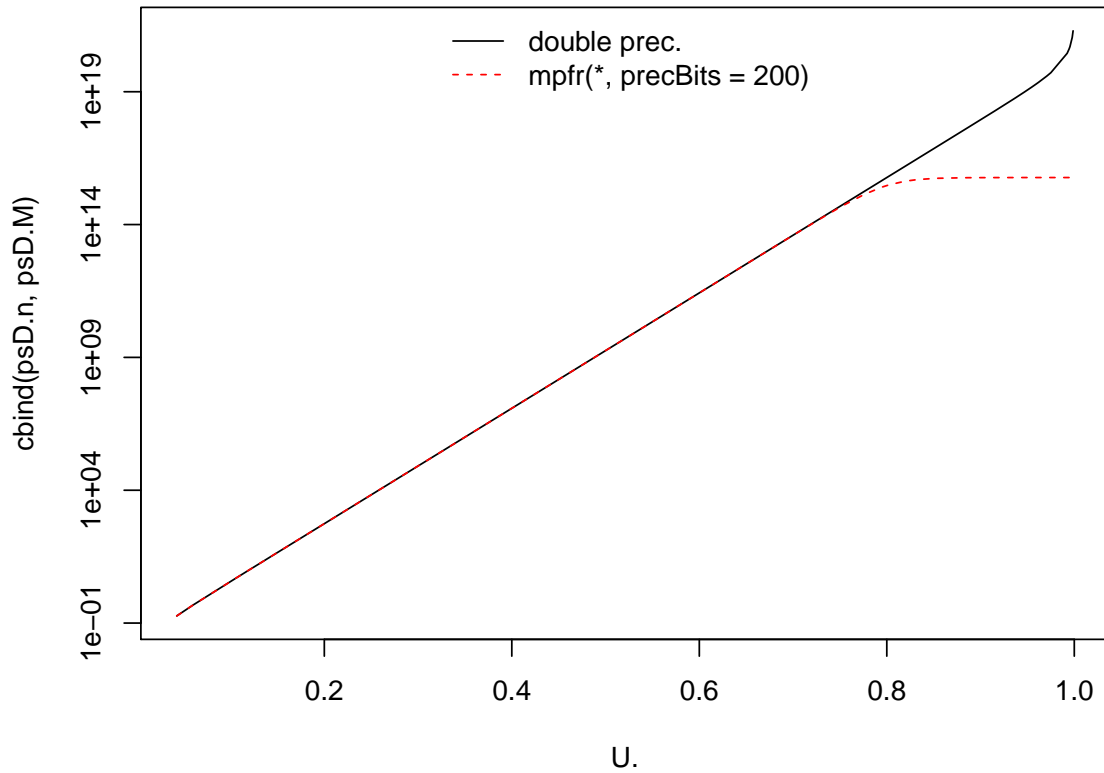
```
psiInv = psiInv.2; psiDabs = psiDabs.2; psiInvDlabs = psiInvDlabs.1
```

where we have already tried to ensure that the `psiInv()` function is ok, but now can confirm it, e.g., for $\theta = 50$. Further note, that using high-precision arithmetic, we can also “partially afford” to use the simplistic `psiInv.0()` function instead the more stable `psiInv.2()` one:

```
> stopifnot(all.equal(psiInv.2(U., 50),
                      psiInv.2(U., mpfr(50, 96))),
             all.equal(psiInv.0(U., mpfr(50, 200)),
                       pI.U <- psiInv.2(U., mpfr(50, 200)), tol=1e-50) )
```

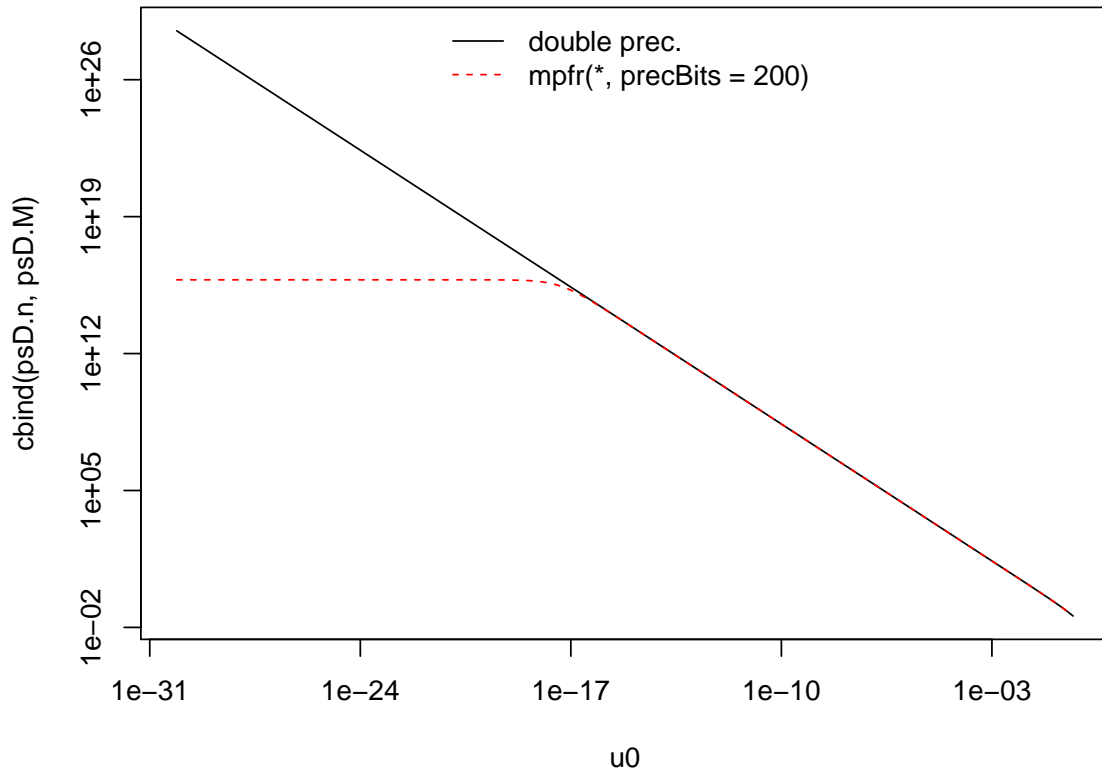
However, we can observe dramatic differences in `psiDabs.2()` ($= |\psi'(\cdot)|$):

```
> psD.n <- psiDabs.2(as.numeric(pI.U), 40)
> psD.M <- as.numeric(psiDabs.2(pI.U, mpfr(40, 200)))
> matplot(U., cbind(psD.n, psD.M), type="l", log="y")
> legend("top", c("double prec.", "mpfr(*, precBits = 200)"),
        col= 1:2, lty=1:2, bty="n")
```



where we see a very large difference (note the log scale!) for $u \approx 1$, i.e., for very small $p\mathbf{I}.U = \text{psiInv.2}(U., \text{theta}) = \psi_{\theta}^{-1}(u)$.

```
> u0 <- 2^-(100:1)
> psD.n <- psiDabs.2(u0, 40)
> psD.M <- as.numeric(psiDabs.2(u0, mpfr(40, 200)))
> matplot(u0, cbind(psD.n, psD.M), type="l", log="xy")
> legend("top", c("double prec.", "mpfr(*, precBits = 200)"),
       col= 1:2, lty=1:2, bty="n")
```

Further investigation shows that the culprit is really the use of `log(-expm1(-theta))` inside `psiDabs.2()` which underflows for large theta, and hence should be replaced by the generally accurate

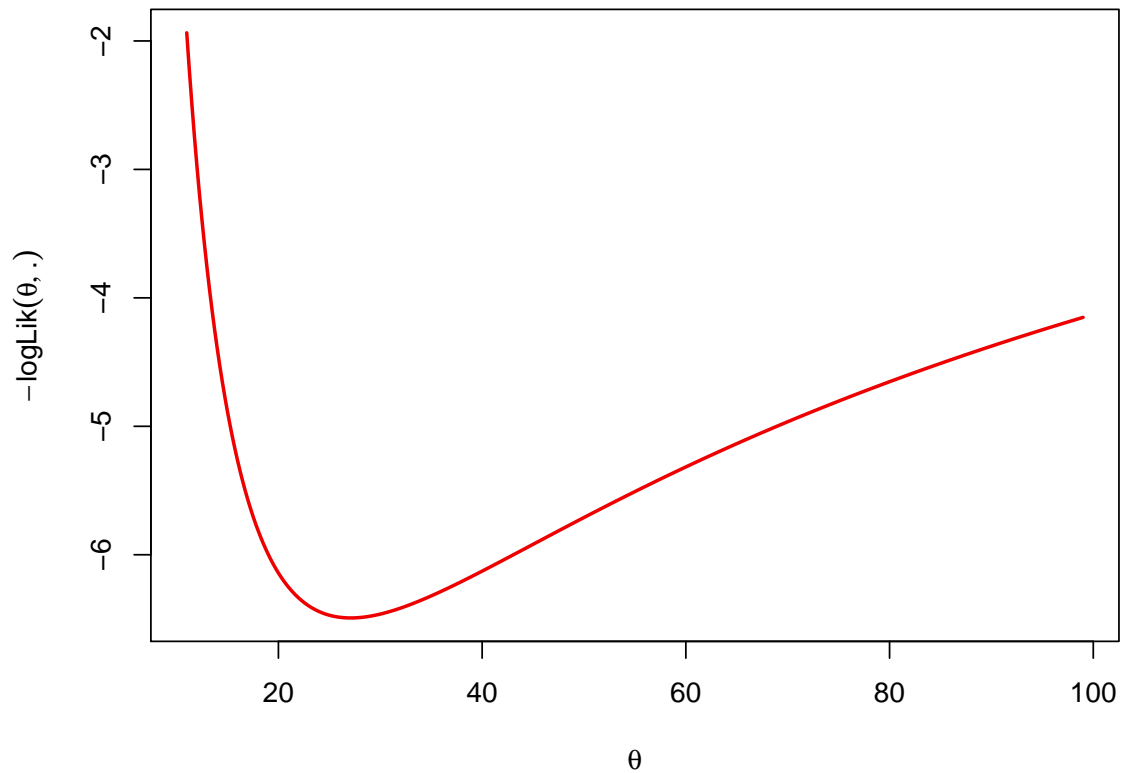
```
> log1mexpm <- function(a)
{
  stopifnot(a >= 0)
  r <- a
  tst <- a <= log(2)
  r[tst] <- log(-expm1(-a[tst]))
  r[!tst] <- log1p(-exp(-a[!tst]))
  r
}
```

so that we rather compute $|\psi'(\cdot)|$ via

```
> psiDabs.3 <- function(t, theta, log=FALSE) {
  w <- log1mexpm(theta) - t
  Li. <- if(log) w - log1mexpm(-w) else -exp(w)/expm1(w)
  if(log) Li. - log(theta) else Li. / theta
}
```

Does this already solve the “diagonal likelihood” problem? We investigate via the graphic

```
> p.mlogL(th = seq(11, 99, by = 1/4),
  mlogL = (mlogL2 <- function(theta)
    -sum(dDiagA(U., theta, d=d, psiInv = psiInv.2,
      psiDabs = psiDabs.3, psiInvD1abs=psiInvD1abs.1,
      log = TRUE))), lwd = 2)
```



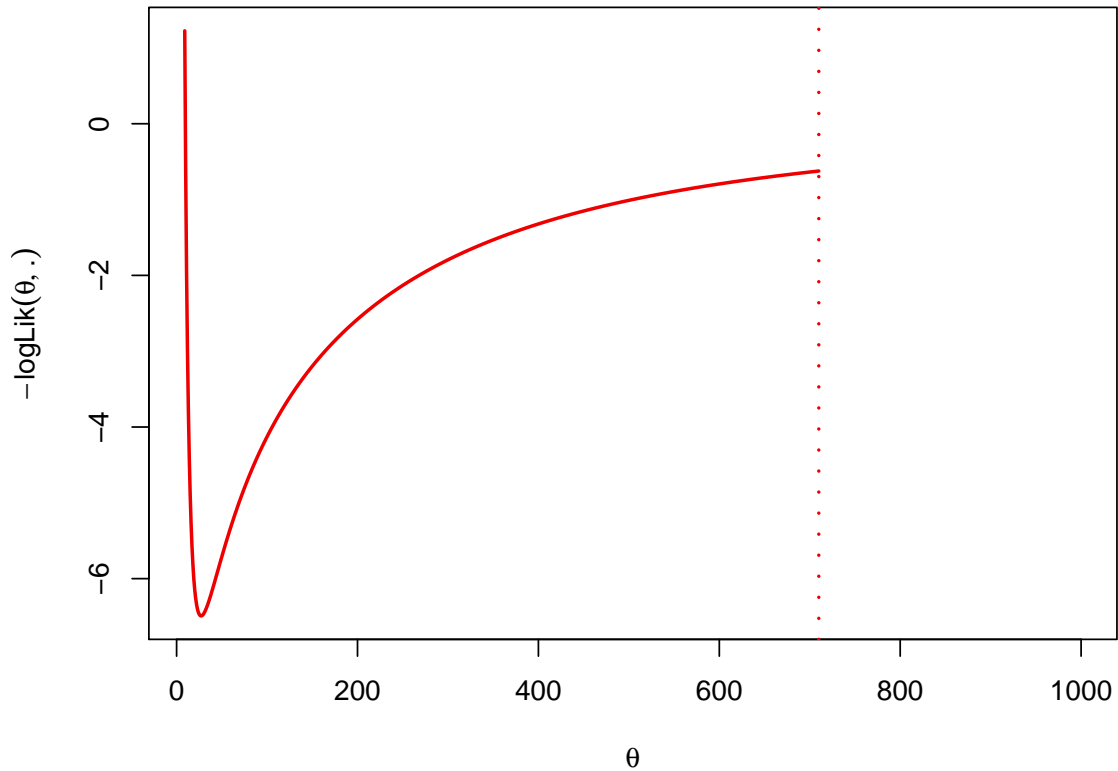
Yes, indeed, using a numerically stable version for `psiDabs()` did solve the numerical problem of computing, the “diagonal likelihood”, and hence the `dmle()` (“diagonal MLE”).

Well, if we really insist, there are more problems, but probably not really practical:

```
> thet <- 9:1000
> nll <- p.mlogL(thet, mlogL = mlogL2, lwd=2)
> (th0 <- thet[i0 <- max(which(is.finite(nll)))])
```

```
[1] 710
```

```
> abline(v = th0, col="red2", lty="15", lwd=2)
```



where we see that for $\theta > 710$, `mlogL()` is not finite, e.g.,

```
> dDiagA(0.999, 715, d = d, psiInv = psiInv.2, psiDabs = psiDabs.3,
          psiInvDlabs = psiInvDlabs.1, log = TRUE)
```

```
[1] -Inf
```

which after closer inspection is from the `psiInvDlabs(u, th, log = TRUE)` part of `dDiagA()` and that, see (6), uses `log(theta)-log(expm1(u*theta))`, where clearly already `expm1(u*theta)` = `expm1(0.999 * 715)` numerically overflows to `Inf`:

```
> psiInvDlabs.1(0.999, th = 715, log=TRUE)
```

```
[1] -Inf
```

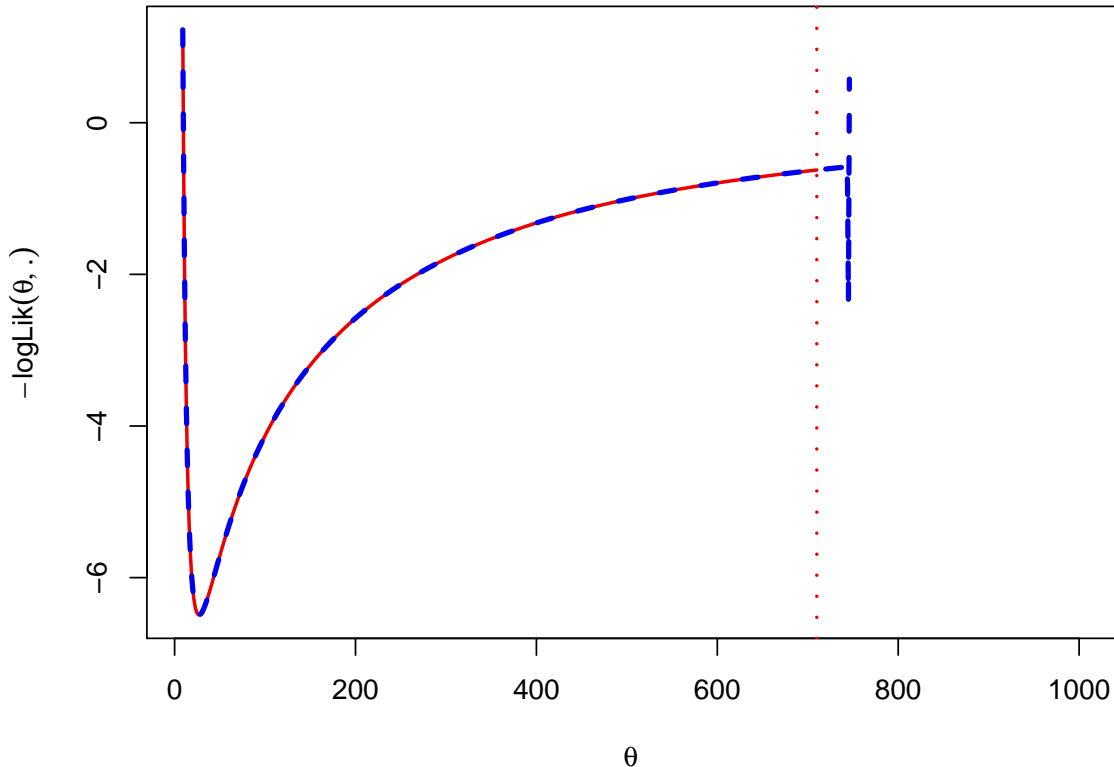
However, as $\log(\expm1(y)) = \log(e^y - 1) = \log(e^y(1 - e^{-y})) = y + \log(1 - e^{-y})$, the “numerical stable” solution is to replace `log(expm1(y))` by `y + log1mexpm(y)`, such that we will use

```
> psiInvDlabs.2 <- function(u, theta, log = FALSE)
  if(log) log(theta)- {y <- u*theta; y + log1mexpm(y)} else theta/expm1(u*theta)
```

Unfortunately, this improves the situation for large θ only slightly:

```
> plot(nll ~ thet, xlab=expression(theta),
       ylab = expression(- logLik(theta, .)),
       type = "l", col="red2", lwd=2)
> abline(v = th0, col="red2", lty="15", lwd=2)
> nll3 <- p.mlogL(thet, mlogL = function(theta)
  -sum(dDiagA(U., theta, d=d, psiInv= psiInv.2, psiDabs= psiDabs.3,
             psiInvDlabs = psiInvDlabs.2, log = TRUE)),
  col = "blue2", lwd=3, lty=2, add = TRUE)
```

```
> nll3[thet == 800]
[1] -Inf
```



where we can see, that this time, the numerical overflow to $-\infty$ happens in `psiDabs(d*psiInv(u,th), th, log = TRUE)`, as `psiInv(u,th) = psiInv(0.999, th=800)=0` underflows to zero — by necessity: the correct value is smaller than the smallest representable double precision number:

```
> pI <- psiInv.2(u=0.999, th= mpfr(800, 200))
> cat(sapply(list(pI, .Machine$double.xmin),
              format, digits = 7), "\n")
4.495130e-348 2.225074e-308
```

The only solution here is to allow passing the *logarithm* $\log(t)$ instead of t to `psiDabs()`, i.e., we start computing `log(psiInv(.))` directly (evading the underflow to 0 there).

.....to be continued.

3. Session Information

```
> toLatex(sessionInfo())
```

- R Under development (unstable) (2012-04-10 r58965), x86_64-unknown-linux-gnu
- Locale: LC_CTYPE=de_CH.UTF-8, LC_NUMERIC=C, LC_TIME=en_US.UTF-8, LC_COLLATE=C, LC_MONETARY=en_US.UTF-8, LC_MESSAGES=C, LC_PAPER=C, LC_NAME=C,

```
LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=de_CH.UTF-8,  
LC_IDENTIFICATION=C
```

- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: Rmpfr 0.4-7, copula 0.99-1, gmp 0.5-1, pspline 1.0-14
- Loaded via a namespace (and not attached): ADGofTest 0.3, gsl 1.9-9, mvtnorm 0.9-9992, stabledist 0.6-3, stats4 2.16.0, tools 2.16.0

4. Conclusion

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/people/maechler>