Numerically Stable Frank Copula Functions via Multiprecision: R Package Rmpfr

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Abstract

The package **copula** (formerly **nacopula**) has provided functionality for Archimedean copulas, one of them the "Frank copula". Recently, explicit formulas for the density of those copulas have allowed for maximum likelihood estimation in high (e.g., d = 150)) dimensions, (Hofert, Mächler, and McNeil (2012)).

However for non-small dimensions, the evaluation of these densities is numerically challenging, and in some cases difficult. Here, we use high precision arithmetic from MPFR, via R package **Rmpfr** in order to get accurate values for the diagonal density of the Frank copula.

Subsequently, judiciously analysing and circumventing the numerical infelicities of the "traditional" evaluation, we gain accurate values even with traditional (double precision) arithmetic.

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 $U = (U_1, U_2, \dots, U_d)^{\mathsf{T}} \sim C$. The (cumulative) distribution function, by definition,

$$F^{D}(u) := P\left[\max(U_{1}, U_{2}, \dots, U_{d}) \le u\right] = P\left[U_{1} \le u, U_{2}, \le u, \dots, U_{d} \le u\right] = C(u, u, \dots, u),$$
(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

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

the diagonal density is

$$f^{D}(u) = \frac{d}{du}F^{D}(u) = \frac{d}{du}\psi\left(\sum_{j=1}^{d}\psi^{-1}(u)\right) = \frac{d}{du}\psi(d\cdot\psi^{-1}(u)) =$$

$$= \psi'(d\cdot\psi^{-1}(u))\cdot d\cdot \frac{d}{du}\psi^{-1}(u)$$

$$= d\cdot\psi'(d\cdot\psi^{-1}(u))\cdot [\psi^{-1}]'(u).$$
(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] \leftarrow dDiagA(u[!i0], d = d, cop = cop, log = log)
        return(u)
    }
    if (log) {
        log(d) + cop@absdPsi(d * cop@iPsi(u, th), th, log = TRUE) +
            cop@absdiPsi(u, th, log = TRUE)
    }
    else {
        d * cop@absdPsi(d * cop@iPsi(u, th), th) * cop@absdiPsi(u,
    }
}
<bytecode: 0x5635f10d8bf0>
```

where the three functions

$$absdPsi(t, thet) = |\psi'_{\theta}(t)|, \tag{4}$$

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

$$absdiPsi(u, thet) = \left| [\psi_{\theta}^{-1}]'(u) \right| \tag{6}$$

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,

Now, for the Frank copula (Hofert and Maechler (2011)),

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

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

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

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

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

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

$$polylog(z, s = 0) = Li_0(z) = z/(1-z).$$
 (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 iPsi.0(u, th) for $\psi_{\theta}^{-1}(u)$ by iPsi.1(), making use of expm1(). These and the derivative (10) originally were

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

```
> absdPsi.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
}</pre>
```

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 u_1, u_2, \ldots, u_n , $(u_i \in [0, 1]^d)$ is

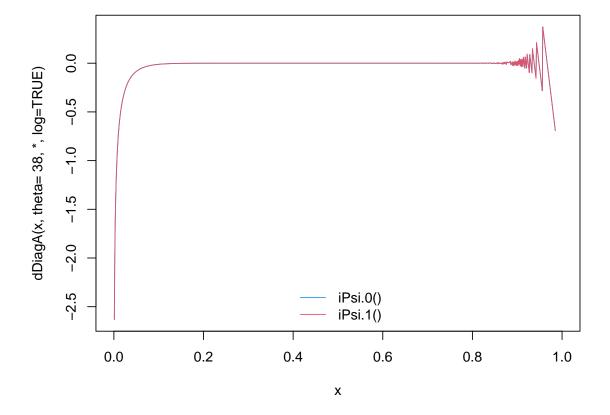
defined as minimizer of the negative log-likelihood,

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

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

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

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

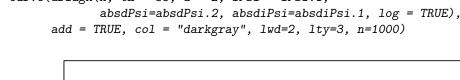


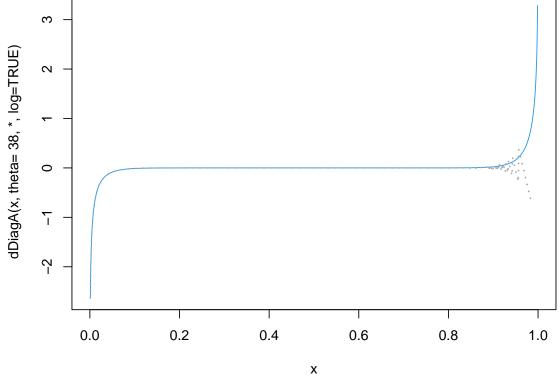
However, it's not hard to see that indeed our initial computation of Frank's ψ_{θ}^{-1} , i.e, (8), $\psi_{\theta}^{-1}(u) = -\log\left(\frac{1-e^{-u\theta}}{1-e^{-\theta}}\right)$, suffers from "division cancellation" for "large" θ ($\theta = 38$ in ex.) when computed directly with iPsi.0(), see above,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

instead of exp(-t) - 1, as used in iPsi.1(), see above, helps only for $t \approx 0$. However, we can rewrite ψ_{θ}^{-1} as

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

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





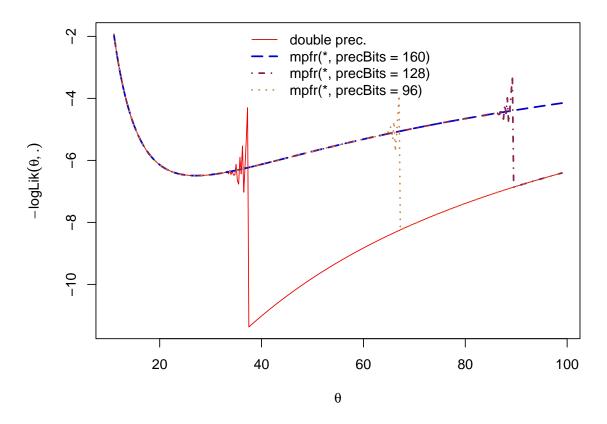
Unfortunately, this is not enough to get numerically stable evaluations of the negative log-likelihood l():

```
> d <- 5
> (theta <- copFrank@iTau(tau = 0.75))

[1] 14.13852
> 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</pre>
```

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.)</pre>
    if(add) lines(nll ~ th, col=col, lwd=lwd, lty=lty)
    else plot(nll ~ th, xlab=expression(theta),
               ylab = expression(- logLik(theta, .)),
               type = "1", 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 ...
> ## using three different precisions:
> MPrecBits <- c(160, 128, 96)
> mkNm <- function(bits) sprintf("%03d.bits", bits)</pre>
> ## As it takes a while, cache the result:
> fnam <- sprintf("mlogL_mpfr_%s.rds", Sys.info()[["machine"]])</pre>
> if(file.exists(fn <- file.path(copDDir, fnam))) {</pre>
      nllMP <- readRDS(fn)</pre>
  } else {
      print(system.time(
      nllMP <- lapply(MPrecBits, function(pBit) {</pre>
          nlM <- thM <- mpfr(thet, precBits = pBit)</pre>
          ## (vapply() does not work for "Rmpfr":)
          for(i in seq_along(thet)) nlM[i] <- mlogL(thM[i])</pre>
      7)
    )) ## ~ 18 sec [R 3.5.1 nb-mm4 core I7vPro]; was 91 sec [2011-06-14 nb-mm icore 5]
    names(nllMP) <- mkNm(MPrecBits)</pre>
    copSrcDDir <- if(Sys.getenv("USER") == "maechler")</pre>
         '~/R/Pkgs/copula/inst/doc' else ""
    if(file.exists(copSrcDDir))# <<- only for certain users; not on CRAN etc
        saveRDS(n11MP, file = file.path(copSrcDDir, fnam), version = 2)
> colB <- c("blue3", "violetred4", "tan3")</pre>
> 1 tyB <- c(5:3)
> 1 \text{wdB} < - c(2,2,2)
> for(i in seq_along(nl1MP)) {
      lines(thet, as.numeric(nllMP[[i]]),
            col=colB[i], lty = ltyB[i], lwd = lwdB[i])
> leg <- c("double prec.", sprintf("mpfr(*, precBits = %d)", MPrecBits))</pre>
> 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

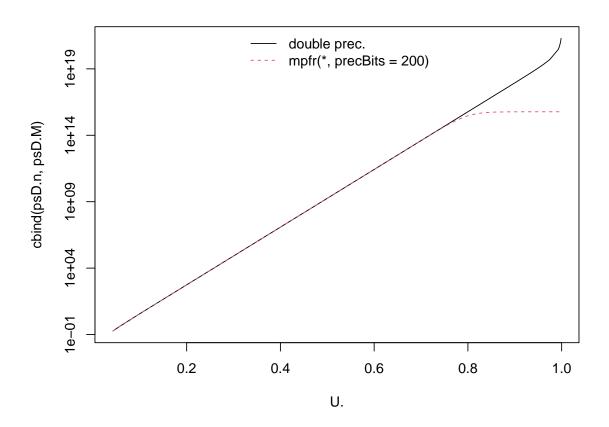
```
absdPsi(d*iPsi(u,th), th, log = TRUE) +
absdiPsi(u, th, log = TRUE)
```

currently, with the three functions

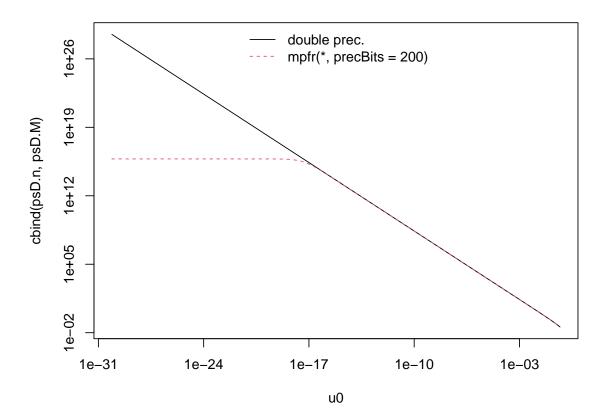
```
iPsi = iPsi.2; absdPsi = absdPsi.2; absdiPsi = absdiPsi.1
```

where we have already tried to ensure that the iPsi() 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 iPsi.0() function instead of the more stable iPsi.2() one:

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

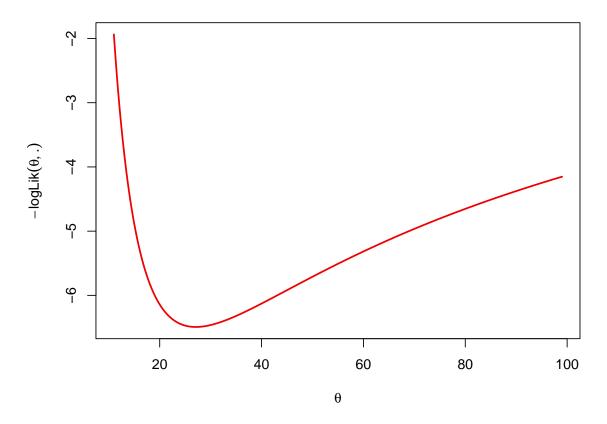


where we see a very large difference (note the log scale!) for $u\approx 1$, i.e., for very small pI.U= iPsi.2(U., theta)= $\psi_{\theta}^{-1}(u)$.



Further investigation shows that the culprit is really the use of log(-expm1(-theta)) inside absdPsi.2() which underflows for large theta, and hence should be replaced by the generally accurate log1mexp(), see Mächler (2012).

```
> log1mexp <- function(a) # accurately compute log(1-exp(-a))</pre>
  {
      stopifnot(a >= 0)
      r <- a
      tst <- a <= log(2)
      r[tst] \leftarrow log(-expm1(-a[tst]))
      r[!tst] \leftarrow log1p(-exp(-a[!tst]))
  }
so that we rather compute |\psi'(.)| via
> absdPsi.3 <- function(t, theta, log=FALSE) {</pre>
    w <- log1mexp(theta) - t</pre>
    Li. <- if(log) w - log1mexp(-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)</pre>
                     -sum(dDiagA(U., theta, d=d, iPsi = iPsi.2,
                                 absdPsi = absdPsi.3, absdiPsi=absdiPsi.1,
                                 log = TRUE))), lwd = 2)
```



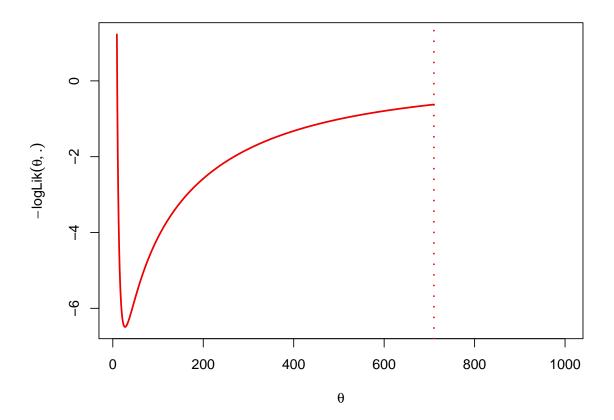
Yes, indeed, using a numerically stable version for absdPsi() did solve the numerical problem of computing, the "diagonal likelihood", and hence the dmle() ("diagonal MLE").

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)))])</pre>
```

[1] 710

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

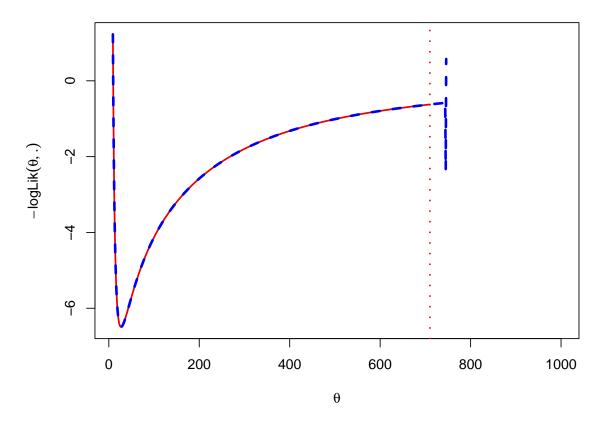


```
where we see that for \theta > 710, mlogL() is not finite, e.g.,
> dDiagA(0.999, 715, d = d, iPsi = iPsi.2, absdPsi = absdPsi.3,
                              absdiPsi = absdiPsi.1, log = TRUE)
[1] -Inf
which after closer inspection is from the absdiPsi(u, th, log = TRUE) part of dDiagA()
and that, see (6), uses log(theta)-log(expm1(u*theta)), where clearly already expm1(u*theta))
= expm1(0.999 * 715) numerically overflows to Inf:
> absdiPsi.1(0.999, th = 715, log=TRUE)
[1] -Inf
However, as \log(\exp(1/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 + log1mexp(y), such that we will use
> absdiPsi.2 <- function(u, theta, log = FALSE)</pre>
    if(log) log(theta) - {y <- u*theta; y + log1mexp(y)} else theta/expm1(u*theta)
Unfortunately, this improves the situation for large \theta only slightly:
> plot(nll ~ thet, xlab=expression(theta),
       ylab = expression(- logLik(theta, .)),
       type = "1", col="red2", lwd=2)
> abline(v = th0, col="red2", lty="15", lwd=2)
> nl13 <- p.mlogL(thet, mlogL = function(theta)</pre>
                    -sum(dDiagA(U., theta, d=d, iPsi= iPsi.2, absdPsi= absdPsi.3,
                                 absdiPsi = absdiPsi.2, log = TRUE)),
```

col = "blue2", lwd=3, lty=2, add = TRUE)

> n113[thet == 800]

[1] -Inf



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

4.495130e-348 2.225074e-308

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

..... to be continued.

3. Session Information

> toLatex(sessionInfo())

- R version 4.0.3 Patched (2020-12-08 r79596), x86_64-pc-linux-gnu
- Locale: LC_CTYPE=en_US.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=en_US.UTF-8,

- $\label{lc_name} \mbox{LC_NAME=C, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=en_US.UTF-8, LC_IDENTIFICATION=C}$
- Running under: Debian GNU/Linux bullseye/sid
- Matrix products: default
- BLAS: /srv/R/R-patched/build.20-12-10/lib/libRblas.so
- LAPACK: /srv/R/R-patched/build.20-12-10/lib/libRlapack.so
- Base packages: base, datasets, grDevices, graphics, grid, methods, parallel, splines, stats, stats4, tools, utils
- Other packages: Rmpfr 0.8-2, VGAM 1.1-4, abind 1.4-5, bbmle 1.0.23.1, copula 1.0-1, gmp 0.6-1, gridExtra 2.3, gsl 2.1-6, lattice 0.20-41, mev 1.13.1, qrng 0.0-8, randtoolbox 1.30.1, rngWELL 0.10-6, rugarch 1.4-4, sfsmisc 1.1-7
- Loaded via a namespace (and not attached): ADGofTest 0.3, DistributionUtils 0.6-0, GeneralizedHyperbolic 0.8-4, KernSmooth 2.23-18, MASS 7.3-53, Matrix 1.2-18, Rcpp 1.0.5, Rsolnp 1.16, Runuran 0.33, SkewHyperbolic 0.4-0, TruncatedNormal 2.2, alabama 2015.3-1, bdsmatrix 1.3-4, boot 1.3-25, compiler 4.0.3, digest 0.6.27, evaluate 0.14, evd 2.3-3, gtable 0.3.0, htmltools 0.5.0, knitr 1.30, ks 1.11.7, magrittr 2.0.1, mclust 5.4.7, mvtnorm 1.1-1, nleqslv 3.3.2, nloptr 1.2.2.2, numDeriv 2016.8-1.1, partitions 1.9-22, pcaPP 1.9-73, polynom 1.4-0, pspline 1.0-18, rlang 0.4.9, rmarkdown 2.5, spd 2.0-1, stabledist 0.7-1, stringi 1.5.3, stringr 1.4.0, truncnorm 1.0-8, xfun 0.19, xts 0.12.1, yaml 2.2.1, zoo 1.8-8

4. Conclusion

References

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