

Negative Binomial factor regression with application to microbiome data analysis

Aditya Mishra, Christian L. Müller

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```
library(nbfar)
```

Simulation examples

We showcase the usage of **nbfar** and **nbrrr** on simulated data. We simulate response and covariates matrix for multivariate negative binomial regression with a low-rank and sparse coefficient matrix. The coefficient matrix \mathbf{C} is expressed in terms of \mathbf{U} (left singular vector), \mathbf{D} (singular values) and \mathbf{V} (right singular vector).

Data simulation

```
## ## -----Simulation settings -----
## Simulation setting:
## n: sample size
## p: number of predictors
## pz: number of control variable other than intercept parameter
## q: number of outcome variables
## nrank: true rank of the model
## snr: signal to noise ratio to be used in generating gaussian outcome variables
## nlam: number of lambda values to be fitted
## rank.est: maximum estimated rank to be specified to the model
## s: multiplicative factor of singular values
## nthread: number of parallel thread can be used in parallel for cross validation
## The simulation was replicated 100 times under each setting as detailed in the paper.

#
## Model specification:
p <- 50;
example_seed <- 123
xp = 30
set.seed(example_seed)
n <- 200
nrank <- 3           # true rank
rank.est <- 5       # estimated rank
nlam <- 40          # number of tuning parameter
s = 0.5; q <- 30
sp = xp/p
nthread = 1
```

```

## ----- Generate low-rank and sparse coefficient matrix ---
## D: singular values
## U: sparse left singular vectors
## V: sparse right singular vectors
D <- rep(0, nrank)
V <- matrix(0, ncol = nrank, nrow = q)
U <- matrix(0, ncol = nrank, nrow = p)
#
U[, 1] <- c(sample(c(1, -1), 8, replace = TRUE), rep(0, p - 8))
U[, 2] <- c(rep(0, 5), sample(c(1, -1), 9, replace = TRUE), rep(0, p - 14))
U[, 3] <- c(rep(0, 11), sample(c(1, -1), 9, replace = TRUE), rep(0, p - 20))
#
# for similar type response type setting
V[, 1] <- c(rep(0, 8), sample(c(1, -1), 8, replace = TRUE) *
            runif(8, 0.3, 1), rep(0, q - 16))
V[, 2] <- c(rep(0, 20), sample(c(1, -1), 8, replace = TRUE) *
            runif(8, 0.3, 1), rep(0, q - 28))
V[, 3] <- c( sample(c(1, -1), 5, replace = TRUE) *
            runif(5, 0.3, 1), rep(0, 23),
            sample(c(1, -1), 2, replace = TRUE) *
            runif(2, 0.3, 1), rep(0, q - 30))
U[, 1:3] <- apply(U[, 1:3], 2, function(x) x / sqrt(sum(x^2)))
V[, 1:3] <- apply(V[, 1:3], 2, function(x) x / sqrt(sum(x^2)))
#
D <- s * c(4, 6, 5) # signal strength varries as per the value of s
or <- order(D, decreasing = T)
U <- U[, or]
V <- V[, or]
D <- D[or]
C <- U %*% (D * t(V)) # simulated coefficient matrix
intercept <- rep(0.5, q) # specifying intercept to the model:
C0 <- rbind(intercept, C)

## ----- Simulate data -----
Xsigma <- 0.5^abs(outer(1:p, 1:p, FUN = "-"))
sim.sample <- nbfar_sim(U, D, V, n, Xsigma, C0, disp = 0.75, depth = 10) # Simulated sample
X <- sim.sample$X[1:n, ] # simulated predictors (training)
Y <- sim.sample$Y[1:n, ] # simulated responses (training)
# 1000 test sample data
sim.sample <- nbfar_sim(U, D, V, 1000, Xsigma, C0, disp = 0.75, depth = 10)
Xt <- sim.sample$X # simulated predictors (test)
Yt <- sim.sample$Y # simulated predictors (test)
X0 <- cbind(1, X) # 1st column accounting for intercept

# Simulate data with 20% missing entries
miss <- 0.10 # Proportion of entries missing
t.ind <- sample.int(n * q, size = miss * n * q)
y <- as.vector(Y)
y[t.ind] <- NA
Ym <- matrix(y, n, q) # 20% of entries are missing at random

```

Negative Binomial reduced rank regression: nbrrr

In the range of 1 to maxrank, the estimation procedure selects the rank r of the coefficient matrix using a cross-validation approach. For the selected rank, a rank r coefficient matrix is estimated that best fits the observations.

```
# Model fit: (full data)
set.seed(example_seed)
control_r3 <- nbfar_control(initmaxit = 10000, initepsilon = 1e-5,
                           objI = 1)
# nbrrr_test <- nbrrr(Y, X, maxrank = 5, control = control_r3, nfold = 5, trace = F)

# Model fit: (missing data)
set.seed(example_seed)
control_r3 <- nbfar_control(initmaxit = 10000, initepsilon = 1e-5,
                           objI = 1)
# nbrrr_testm <- nbrrr(Ym, X, maxrank = 5, control = control_r3, nfold = 5, trace = F)
```

Negative Binomial co-sparse factor regression: nbfar

To estimate a low-rank and sparse coefficient matrix in large/high dimensional setting, the approach extracts unit-rank components of required matrix in sequential order. The algorithm automatically stops after extracting sufficient unit rank components.

```
# Model fit: (full data)
RcppParallel::setThreadOptions(numThreads = nthread)
set.seed(example_seed)
control_nbfar <- nbfar_control(gamma0 = 1, spU = sp, spV = 20/q,
                              maxit = 2000, lamMaxFac = 1e-2,
                              lamMinFac = 1e-7, epsilon = 1e-4,
                              objI = 0,
                              initmaxit = 10000, initepsilon = 1e-7)
# nbfar_test <- nbfar(Y, X, maxrank = rank.est, nlambda = nlam,
#                   cIndex = NULL,
#                   ofset = NULL, control = control_nbfar, nfold = 5,
#                   PATH = FALSE, nthread = nthread, trace = F)

# Model fit: (missing data)
RcppParallel::setThreadOptions(numThreads = nthread)
set.seed(example_seed)
control_nbfar <- nbfar_control(gamma0 = 1, spU = sp, spV = 20/q,
                              maxit = 2000, lamMaxFac = 1e-2,
                              lamMinFac = 1e-7, epsilon = 1e-4,
                              objI = 0,
                              initmaxit = 10000, initepsilon = 1e-7)
# nbfar_testm <- nbfar(Ym, X, maxrank = rank.est, nlambda = nlam,
#                   cIndex = NULL,
#                   ofset = NULL, control = control_nbfar, nfold = 5,
#                   PATH = FALSE, nthread = nthread, trace = F)
```