Package 'nnsolve'

March 24, 2026

Type Package

Title Fast Non-Negative Least Squares

Version 0.0.1

Date 2026-03-11

Description Provides a fast algorithm for solving non-negative least squares problems. It implements the Fast Non-Negative Least Squares algorithm of Bro and de Jong (1997) <doi:10.1002/(SICI)1099-128X(199709/10)11:5%3C393::AID-CEM483%3E3.0.CO;2-L>.

License GPL (>= 2)

Imports Rcpp (>= 1.1.1)

LinkingTo Rcpp, RcppEigen

RoxygenNote 7.3.3

Encoding UTF-8

Suggests testthat (>= 3.0.0)

Config/testthat/edition 3

NeedsCompilation yes

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Repository CRAN

Date/Publication 2026-03-24 08:50:02 UTC

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`fnnls` *Fast Non-Negative Least Squares*

Description

Solves the NNLS problem min ||Xty - XtX * w||^2 subject to w >= 0 using the Fast Non-Negative Least Squares algorithm of Bro & de Jong (1997).

Usage

```
fnnls(
  XtX,
  Xty,
  tol = 1e-06,
  max_iter = 1000,
  sum_to_constant = FALSE,
  constant = 1,
  lower_bound = FALSE,
  lb = 0
)
```

Arguments

`XtX`	symmetric positive definite matrix of dimensions k x k
`Xty`	numeric vector of length k
`tol`	convergence tolerance. Default 1e-6
`max_iter`	maximum number of iterations. Default 1000
`sum_to_constant`	if TRUE all entries sum to 'constant'.Default FALSE
`constant`	if sum_to_constant is TRUE, all entries sum to this number. Default 1
`lower_bound`	if TRUE all entries bounded below by 'lb', otherwise they are nonnegative. Default FALSE
`lb`	if lower_bound is TRUE all entries are bounded below by 'lb'. Default 0

Value

non-negative numeric vector of length k

References

Bro, Rasmus & Jong, Sijmen. (1997). A Fast Non-negativity-constrained Least Squares Algorithm. Journal of Chemometrics. 11. 393-401. 10.1002/(SICI)1099-128X(199709/10)11:53.0.CO;2-L.

Examples

```
k <- 10
D <- 100
H   <- matrix(rnorm(k * D), nrow = k, ncol = D)
x   <- rnorm(D)
XtX <- H %*% t(H) + diag(1e-8, k)
Xty <- as.vector(H %*% x)
w   <- fnnls(XtX, Xty)
```

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