Package: nnsolve (via r-universe)

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Type Package

Title Fast Non-Negative Least Squares

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Description This package 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).

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Imports Rcpp, Rfast

LinkingTo Rcpp, RcppEigen

RoxygenNote 7.3.3

Encoding UTF-8

Config/pak/sysreqs make

Repository https://nikolas-kk.r-universe.dev

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RemoteUrl https://github.com/nikolas-kk/nnsolve

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Contents

`fnnls` *Fast Non-Negative Least Squares*

Description

Solves the NNLS problem min ||y - x * 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)
```

`fnnls_reg` *Fast Non-Negative Least Squares Regression*

Description

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

Usage

```
fnnls_reg(
  y,
  X,
  tol = 1e-06,
  max_iter = 1000,
  sum_to_constant = FALSE,
  constant = 1,
  lower_bound = FALSE,
  lb = 0
)
```

Arguments

`y`	A numeric vector of length n.
`X`	A numeric matrix of dimensions n x k.
`tol`	The convergence tolerance, default is 1e-6.
`max_iter`	The maximum number of iterations, default is 1000.
`sum_to_constant`	If TRUE all entries sum to 'constant', Default is FALSE.
`constant`	If sum_to_constant is TRUE, all entries sum to this number. The default value is 1.
`lower_bound`	If TRUE all entries bounded below by 'lb', otherwise they are nonnegative. The default value is FALSE.
`lb`	If lower_bound is TRUE all entries are bounded below by 'lb'. The default value is 0.

Value

A list with two elements:

- b: A non-negative numeric vector of length k with the estimated coefficients.
- mse: The mean squared error of the fitted model.

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

```
n <- 100
k <- 10
X <- matrix(rnorm(n * k), nrow = n, ncol = k)
true_b <- abs(rnorm(k))
y <- X %*% true_b + rnorm(n, sd = 0.1)
result <- fnnls_reg(y, X)
result$b
result$mse
```

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fnnls_regs *Fast Non-Negative Least Squares for Multiple Outputs*

Description

Solves the NNLS problem min ||Y - XB||_F^2 subject to B >= 0 using the Fast Non-Negative Least Squares algorithm of Bro & de Jong (1997).

Usage

```
fnnls_regs(
  Y,
  X,
  tol = 1e-06,
  max_iter = 1000,
  sum_to_constant = FALSE,
  constant = 1,
  lower_bound = FALSE,
  lb = 0,
  parallel = FALSE,
  ncores = -1
)
```

Arguments

Y	A numeric matrix of dimensions n x m.
X	A numeric matrix of dimensions n x p.
tol	The convergence tolerance, default is 1e-6.
max_iter	The maximum number of iterations, default is 1000.
sum_to_constant	If TRUE all entries in each column of B sum to 'constant'. Default is FALSE.
constant	If sum_to_constant is TRUE, all entries in each column sum to this number. The default value is 1.
lower_bound	If TRUE all entries bounded below by 'lb', otherwise they are nonnegative. The default value is FALSE.
lb	If lower_bound is TRUE all entries are bounded below by 'lb'. The default value is 0.
parallel	If TRUE, the columns of B are computed in parallel. The default value is FALSE.
ncores	If parallel is TRUE, this many cores are used in the parallel computations. Must be positive integer. The default value is -1 (use all available cores).

Value

A list with two elements:

- B: A non-negative numeric matrix of dimensions p x m with the estimated coefficients.
- mse: A numeric vector of length m with the mean squared error for each output column.

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

```
n <- 50
p <- 10
m <- 3
X <- matrix(rnorm(n * p), nrow = n, ncol = p)
Y <- matrix(runif(n * m, min = 0, max = 10), nrow = n, ncol = m)
result <- fnnls_regs(Y, X, tol = 1e-8, max_iter = 1000)
result$B
result$mse
```

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