Package 'isotone'

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Type Package Title Active Set and Generalized PAVA for Isotone Optimization Version 1.1-2 Date 2025-05-21 Author Patrick Mair [aut, cre], Jan De Leeuw [aut], Kurt Hornik [aut] Maintainer Patrick Mair <mair@fas.harvard.edu> Description Contains two main functions: one for solving general isotone regression problems using the pool-adjacent-violators algorithm (PAVA); another one provides a framework for active set methods for isotone optimization problems with arbitrary order restrictions. Various types of loss functions are prespecified. Imports graphics, stats, nnls **Depends** R (>= 3.0.2) License GPL-2 URL https://r-forge.r-project.org/projects/psychor/ LazyData yes LazyLoad yes ByteCompile yes NeedsCompilation no **Repository** CRAN Date/Publication 2025-05-22 05:25:19 UTC

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activeSet

Active Set Methods for Isotone Optimization

Description

Isotone optimization can be formulated as a convex programming problem with simple linear constraints. This functions offers active set strategies for a collection of isotone optimization problems pre-specified in the package.

Usage

```
activeSet(isomat, mySolver = "LS", x0 = NULL, ups = 1e-12, check = TRUE,
maxiter = 100, ...)
```

Arguments

| isomat | Matrix with 2 columns that contains isotonicity conditions, i.e. for row i it holds that fitted value i column 1 <= fitted value i column 2 (see examples) |
|----------|--|
| mySolver | Various functions are pre-defined (see details). Either to function name or the corresponding string equivalent can be used. For user-specified functions fSolver with additional arguments can be used (see details as well). |
| ×0 | Feasible starting solution. If NULL the null-vector is used internally. |
| ups | Upper boundary |
| check | If TRUE, KKT feasibility checks for isotonicity of the solution are performed |
| maxiter | Iteration limit |
| | Additional arguments for the various solvers (see details) |

activeSet

Details

The following solvers are specified. Note that y as the vector of observed values and weights as the vector of weights need to provided through ... for each solver (except for fSolver() and sSolver()). Some solvers need additional arguments as described in the corresponding solver help files. More technical details can be found in the package vignette.

The pre-specified solvers are the following (we always give the corresponding string equivalent in brackets): lsSolver() ("LS") for least squares with diagonal weights, aSolver() ("asyLS") for asymmetric least squares, dSolver() ("L1") for the least absolute value, eSolver() ("L1eps") minimizes 11-approximation. hSolver() ("huber") for Huber loss function, iSolver() ("SILF") for SILF loss (support vector regression), lfSolver() ("GLS") for general least squares with non-diagonal weights, mSolver() ("chebyshev") for Chebyshev L-inf norm, oSolver() ("Lp") for L-p power norm, pSolver() ("quantile") for quantile loss function, and finally sSolver() ("poisson") for Poisson likelihood.

fSolver() for user-specified arbitrary differentiable functions. The arguments fobj (target function) and gobj (first derivative) must be provided plus any additional arguments used in the definition of fobj.

Value

Generates an object of class activeset.

| x | Vector containing the fitted values |
|-------------|---|
| У | Vector containing the observed values |
| lambda | Vector with Lagrange multipliers |
| fval | Value of the target function |
| constr.vals | Vector with the values of isotonicity constraints |
| Alambda | Constraint matrix multiplied by lambda (should be equal to gradient) |
| gradient | Gradient |
| isocheck | List containing the KKT checks for stationarity, primal feasibility, dual feasibil- ity, and complementary slackness (>= 0 means feasible) |
| niter | Number of iterations |
| call | Matched call |

Author(s)

Jan de Leeuw, Kurt Hornik, Patrick Mair

References

de Leeuw, J., Hornik, K., Mair, P. (2009). Isotone optimization in R: Active Set methods and pool-adjacent-violators algorithm. Journal of Statistical Software, 32(5), 1-24.

See Also

```
gpava, lsSolver, dSolver, mSolver, fSolver, pSolver, lfSolver, oSolver, aSolver, eSolver,
sSolver, hSolver, iSolver
```

Examples

```
## Data specification
set.seed(12345)
                             ##normal distributed response values
y <- rnorm(9)
w1 <- rep(1,9)
                             ##unit weights
Atot <- cbind(1:8, 2:9)
                             ##Matrix defining isotonicity (total order)
Atot
## Least squares solver (pre-specified and user-specified)
fit.ls1 <- activeSet(Atot, "LS", y = y, weights = w1)</pre>
fit.ls1
summary(fit.ls1)
fit.ls2 <- activeSet(Atot, fSolver, fobj = function(x) sum(w1*(x-y)^2),
gobj = function(x) 2*drop(w1*(x-y)), y = y, weights = w1)
## LS vs. GLS solver (needs weight matrix)
set.seed(12345)
wvec <- 1:9
wmat <- crossprod(matrix(rnorm(81),9,9))/9</pre>
fit.wls <- activeSet(Atot, "LS", y = y, weights = wvec)</pre>
fit.gls <- activeSet(Atot, "GLS", y = y, weights = wmat)</pre>
## Quantile regression
fit.qua <- activeSet(Atot, "quantile", y = y, weights = wvec, aw = 0.3, bw = 0.7)
## Mean absolute value norm
fit.abs <- activeSet(Atot, "L1", y = y, weights = w1)</pre>
## Lp norm
fit.pow <- activeSet(Atot, "Lp", y = y, weights = w1, p = 1.2)</pre>
## Chebyshev norm
fit.che <- activeSet(Atot, "chebyshev", y = y, weights = w1)</pre>
## Efron's asymmetric LS
fit.asy <- activeSet(Atot, "asyLS", y = y, weights = w1, aw = 2, bw = 1)</pre>
## Huber and SILF loss
fit.hub <- activeSet(Atot, "huber", y = y, weights = w1, eps = 1)</pre>
fit.svm <- activeSet(Atot, "SILF", y = y, weights = w1, beta = 0.8, eps = 0.2)</pre>
## Negative Poisson log-likelihood
set.seed(12345)
yp <- rpois(9,5)
x0 <- 1:9
fit.poi <- activeSet(Atot, "poisson", x0 = x0, y = yp)</pre>
## LS on tree ordering
```

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aSolver

```
Atree <- matrix(c(1,1,2,2,2,3,3,8,2,3,4,5,6,7,8,9),8,2)
Atree
fit.tree <- activeSet(Atree, "LS", y = y, weights = w1)</pre>
## LS on loop ordering
Aloop <- matrix(c(1,2,3,3,4,5,6,6,7,8,3,3,4,5,6,6,7,8,9,9),10,2)
Aloop
fit.loop <- activeSet(Aloop, "LS", y = y, weights = w1)</pre>
## LS on block ordering
Ablock <- cbind(c(rep(1,3),rep(2,3),rep(3,3),rep(4,3),rep(5,3),rep(6,3)),c(rep(c(4,5,6),3),
rep(c(7,8,9),3)))
Ablock
fit.block <- activeSet(Ablock, "LS", y = y, weights = w1)</pre>
## Isotone LS regression using gpava and active set (same results)
pava.fitted <- gpava(y = y)$x</pre>
aset.fitted <- activeSet(Atot, "LS", weights = w1, y = y)$x</pre>
mse <- mean((pava.fitted - aset.fitted)^2)</pre>
mse
```

aSolver

Asymmetric Least Squares

Description

Minimizes Efron's asymmetric least squares regression.

Usage

aSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|--|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector, weights with optional observation weights, weight aw for $y > x$, and weight bw for $y <= x$ |

Details

This function is called internally in activeSet by setting mySolver = aSolver.

dSolver

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

References

Efron, B. (1991). Regression percentiles using asymmetric squared error loss. Statistica Sinica, 1, 93-125.

See Also

activeSet

Examples

```
##Fitting isotone regression using active set
set.seed(12345)
y <- rnorm(9)  ##response values
w <- rep(1,9)  ##unit weights
btota <- cbind(1:8, 2:9) ##Matrix defining isotonicity (total order)
fit.asy <- activeSet(btota, aSolver, weights = w, y = y, aw = 0.3, bw = 0.5)</pre>
```

Description

Solver for the least absolute value norm with optional weights.

Usage

dSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|---|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector and weights with optional observation weights |

Details

This function is called internally in activeSet by setting mySolver = dSolver.

eSolver

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

See Also

activeSet

Examples

eSolver

L1 approximation

Description

Solves an L1 approximation.

Usage

eSolver(z, a, extra)

Arguments

| z | Vector containing observed response |
|-------|---|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector and weights with optional observation weights, eps for the error term |

Details

This function is called internally in activeSet by setting mySolver = eSolver.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

fSolver

See Also

activeSet

Examples

fSolver

User-Specified Loss Function

Description

Specification of a differentiable convex loss function.

Usage

fSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|--|
| а | Matrix with active constraints |
| extra | List with element fobj containing the target function and gobj with the first derivative |

Details

This function is called internally in activeSet by setting mySolver = fSolver. It uses optim() with "BFGS" for optimization.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

See Also

activeSet

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gpava

Examples

```
##Fitting isotone regression using active set (L2-norm user-specified)
set.seed(12345)
y <- rnorm(9)  ##response values
w <- rep(1,9)  ##unit weights
btota <- cbind(1:8, 2:9)  ##Matrix defining isotonicity (total order)
fit.convex <- activeSet(btota, fSolver, fobj = function(x) sum(w*(x-y)^2),
gobj = function(x) 2*drop(w*(x-y)), y = y, weights = w)</pre>
```

```
gpava
```

Generalized Pooled-Adjacent-Violators Algorithm (PAVA)

Description

Pooled-adjacent-violators algorithm for general isotone regression problems. It allows for general convex target function, multiple measurements, and different approaches for handling ties.

Usage

gpava(z, y, weights = NULL, solver = weighted.mean, ties = "primary", p = NA)

Arguments

| Z | Vector of abscissae values |
|---------|--|
| У | Vector or list of vectors of responses |
| weights | Vector of list of vectors of observation weights |
| solver | Either weighted.mean, weighted.median, weighted.fractile, or a user-specified function (see below) |
| ties | Treatment of ties, either "primary", "secondary", or "tertiary" |
| р | Fractile value between 0 and 1 if weighted.fractile is used |

Details

A Pool Adjacent Violators Algorithm framework for minimizing problems like

$$\sum_i \sum_{J_i} w_{ij} f(y_{ij}, m_i)$$

under the constraint $m_1 \leq ... \leq m_n$ with f a convex function in m. Note that this formulation allows for repeated data in each block (i.e. each list element of y, and hence is more general than the usual pava/isoreg ones.

A solver for the unconstrained $\sum_k w_k f(y_k, m) - > min!$ can be specified. Typical cases are $f(y,m) = |y-m|^p$ for p = 2 (solved by weighted mean) and p = 1 (solved by weighted median), respectively.

Using the weighted.fractile solver corresponds to the classical minimization procedure in quantile regression.

The user can also specify his own function foo(y, w) with responses and weights as arguments. It should return a single numerical value.

hSolver

Value

Generates an object of class gpava.

| х | Fitted values |
|--------|---------------------|
| У | Observed response |
| z | Observed predictors |
| W | Weights |
| solver | Convex function |
| call | Matched call |
| р | Fractile value |
| | |

Author(s)

Kurt Hornik, Jan de Leeuw, Patrick Mair

References

de Leeuw, J., Hornik, K., Mair, P. (2009). Isotone Optimization in R: Pool-Adjacent-Violators Algorithm (PAVA) and Active Set Methods. Journal of Statistical Software, 32(5), 1-24.

Examples

```
data(pituitary)
##different tie approaches
gpava(pituitary[,1],pituitary[,2], ties = "primary")
gpava(pituitary[,1],pituitary[,2], ties = "secondary")
gpava(pituitary[,1],pituitary[,2], ties = "tertiary")
##different target functions
gpava(pituitary[,1],pituitary[,2], solver = weighted.mean)
gpava(pituitary[,1],pituitary[,2], solver = weighted.median)
gpava(pituitary[,1],pituitary[,2], solver = weighted.fractile, p = 0.25)
##repeated measures
```

```
data(posturo)
res <- gpava(posturo[,1],posturo[,2:4], ties = "secondary")
plot(res)</pre>
```

hSolver

Huber Loss Function

Description

Solver for Huber's robust loss function.

hSolver

Usage

hSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|--|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector and weights with optional observation weights, and eps |

Details

This function is called internally in activeSet by setting mySolver = hSolver.

Value

| Х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

References

Huber, P. (1982). Robust Statistics. Chichester: Wiley.

See Also

activeSet

iSolver

Description

Minimizes soft insensitive loss function (SILF) for support vector regression.

Usage

iSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|---|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector, weights with optional observation weights, beta between 0 and 1, and $eps > 0$ |

Details

This function is called internally in activeSet by setting mySolver = iSolver.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

References

Efron, B. (1991). Regression percentiles using asymmetric squared error loss. Statistica Sinica, 1, 93-125.

See Also

activeSet

```
##Fitting isotone regression using active set
set.seed(12345)
y <- rnorm(9)  ##response values
w <- rep(1,9)  ##unit weights
eps <- 2
beta <- 0.4</pre>
```

lfSolver

```
btota <- cbind(1:8, 2:9) ##Matrix defining isotonicity (total order)
fit.silf <- activeSet(btota, iSolver, weights = w, y = y, beta = beta, eps = eps)</pre>
```

lfSolver

General Least Squares Loss Function

Description

Solver for the general least squares monotone regression problem of the form (y-x)'W(y-x).

Usage

lfSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|--|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector and weights as weight matrix W which is not necessarily positive definite. |

Details

This function is called internally in activeSet by setting mySolver = lfSolver.

Value

| Х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

See Also

activeSet

lsSolver

Description

Solver for the least squares monotone regression problem with optional weights.

Usage

lsSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|---|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector and weights with optional observation weights |

Details

This function is called internally in activeSet by setting mySolver = lsSolver.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

See Also

activeSet

mendota

Description

This dataset shows the number of freezing days at Lake Mendota measured from November, 23, in the year 1854.

Usage

data(mendota)

Format

A data frame with 12 subjects.

References

Bhattacharyya, G. K., & Klotz, J. H. (1966). The bivariate trend of Lake Mendota. Technical Report No. 98, Department of Statistics, University of Wisconsin.

Barlow, R. E., Bartholomew, D. J., Bremner, J. M., & Brunk, H. D. (1972). Statistical inference under order restrictions: The theory and application of isotonic regression. Chichester: Wiley.

Examples

data(mendota)

mregnn

Regression with Linear Inequality Restrictions on Predicted Values

Description

The package contains three functions for fitting regressions with inequality restrictions: mregnn is the most general one, allowing basically for any partial orders, mregnnM poses a monotone restriction on the fitted values, mregnnP restricts the predicted values to be positive. Monre details can be found below.

Usage

mregnn(x, y, a)
mregnnM(x, y)
mregnnP(x, y)

mregnn

Arguments

| x | Can be a spline basis. |
|---|---------------------------------------|
| У | Response. |
| а | Matrix containing order restrictions. |

Details

These functions solve the problem

$$f(b) = \frac{1}{2}(y - Xb)'(y - Xb)$$

over all b for which $A'Xb \ge 0$. A can be used require the transformation to be non-negative, or increasing, or satisfying any partial order.

Value

| xb | Predicted values. |
|----|-------------------------------|
| lb | Solution of the dual problem. |
| f | Value of the target function |

References

de Leeuw, J. (2015). Regression with Linear Inequality Restrictions on Predicted Values. http: //rpubs.com/deleeuw/78897.

```
## Compute the best fitting quadratic polynomial (in black)
## and monotone quadratic polynomial (in blue)
set.seed(12345)
x <- outer(1:10,1:3,"^")</pre>
x <- apply(x,2,function(x)</pre>
x - mean(x)
x <- apply (x,2,function(x)</pre>
x / sqrt (sum(x ^ 2)))
y <- rowSums(x) + rnorm(10)</pre>
plot(x[,1], y, lwd = 3, col = "RED", xlab = "x", ylab = "P(x)")
o <- mregnnM(x,y)</pre>
lines(x[,1], o$xb, col = "BLUE", lwd = 2)
xb <- drop(x %*% qr.solve(x,y))</pre>
lines(x[,1],xb,col="BLACK", lwd = 2)
## same monotone model through basic mregnn()
difmat <- function (n) {</pre>
  m1 <- ifelse(outer(1:(n - 1),1:n,"-") == -1, 1, 0)</pre>
  m2 <- ifelse(outer(1:(n - 1),1:n,"-") == 0,-1, 0)</pre>
  return (m1 + m2)
}
a <- difmat(nrow(x))
                           ## order restriction
o2 <- mregnn(x, y, a)
```

mSolver

Description

Solver for the Chebyshev norm.

Usage

mSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|---|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector and weights with optional observation weights |

Details

This function is called internally in activeSet by setting mySolver = mSolver.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

See Also

activeSet

oSolver

Lp norm

Description

Solver for Lp-norm.

Usage

oSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|---|
| a | Matrix with active constraints |
| extra | List with element y containing the observed response vector, weights as an optional weight vector, and p as the exponent for the Lp-norm. |

Details

This function is called internally in activeSet by setting mySolver = oSolver.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

See Also

activeSet

```
##Fitting isotone regression
set.seed(12345)
y <- rnorm(9)  ##normal distributed response values
w1 <- rep(1,9)  ##unit weights
Atot <- cbind(1:8, 2:9)  ##Matrix defining isotonicity (total order)
fit.pow <- activeSet(Atot, oSolver, y = y, weights = w1, p = 1.2)</pre>
```

pituitary

Description

The University of Carolina conducted a study in which the size (in mm) of the pituitary fissure was measured on girls between an age of 8 and 14.

Usage

```
data(pituitary)
```

Format

A data frame with 11 subjects.

References

Pothoff, R. F., & Roy, S. N. (1964). A generalized multivariate analysis of variance model useful especially for growth curve problems. Biometrika, 51, 313-326.

Robertson, T., Wright, F. T., & Dykstra, R. L. (1988). Order restricted statistical inference. New York, Wiley.

Examples

data(pituitary)

posturo

Repeated posturographic measures

Description

This dataset represents a subset from the posturographic data collected in Leitner et al. (sensory organisation test SOT).

Usage

```
data(posturo)
```

Format

A data frame with 50 subjects, age as predictor and 3 repeated SOT measures as responses.

References

Leitner, C., Mair, P., Paul, B., Wick, F., Mittermaier, C., Sycha, T., & Ebenbichler, G. (2009). Reliability of posturographic measurements in the assessment of impaired sensorimotor function in chronic low back pain. Journal of Electromyography and Kinesiology, 19(3), 380-390.

Examples

data(posturo)

pSolver

Quantile Regression

Description

Solver for the general p-quantile monotone regression problem with optional weights.

Usage

pSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|---|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector, weights with op- tional observation weights, aw and bw as quantile weights. |

Details

This function is called internally in activeSet by setting mySolver = pSolver. Note that if aw = bw, we get the weighted median and therefore we solved the weighted absolute norm.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

References

Koenker, R. (2005). Quantile regression. Cambridge, MA: Cambridge University Press.

See Also

activeSet

sSolver

Examples

```
##Fitting quantile regression
set.seed(12345)
y <- rnorm(9)  ##response values
w <- rep(1,9)  ##unit weights
btota <- cbind(1:8, 2:9) ##Matrix defining isotonicity (total order)
fit.p <- activeSet(btota, pSolver, weights = w, y = y, aw = 0.3, bw = 0.7)</pre>
```

```
sSolver
```

Negative Poisson Log-Likelihood

Description

Solver for the negative Poisson log-likelihood

Usage

sSolver(z, a, extra)

Arguments

| Z | Vector containing observed response |
|-------|---|
| а | Matrix with active constraints |
| extra | List with element y containing the observed response vector |

Details

This function is called internally in activeSet by setting mySolver = sSolver.

Value

| х | Vector containing the fitted values |
|-----|-------------------------------------|
| lbd | Vector with Lagrange multipliers |
| f | Value of the target function |
| gx | Gradient at point x |

See Also

activeSet

```
##Minimizing Poisson log-liklihood
set.seed(12345)
yp <- rpois(9,5)
Atot <- cbind(1:8, 2:9)  ##Matrix defining isotonicity (total order)
x0 <- 1:9  ##starting values
fit.poi <- activeSet(Atot, sSolver, x0 = x0, y = yp)</pre>
```

weighted.fractile Weighted Median

Description

Computes the weighted fractile of a numeric vector

Usage

weighted.fractile(y, w, p)

Arguments

| У | A numeric vector containing the values whose fractile is to be computed |
|---|---|
| w | A vector of length y giving the weights to use for each element of y |
| р | Fractile specification; value between 0 and 1 |

See Also

weighted.mean, weighted.median

Examples

```
y <- 1:9
w <- c(rep(1,5), rep(2,4))
res <- weighted.fractile(y, w, p = 0.33)</pre>
```

weighted.median Weighted Median

Description

Computes a weighted median of a numeric vector

Usage

weighted.median(y, w)

Arguments

| У | A numeric vector containing the values whose median is to be computed |
|---|---|
| W | A vector of length y giving the weights to use for each element of y |

See Also

weighted.mean,weighted.fractile

weighted.median

Examples

y <- 1:9
w <- c(rep(1,5), rep(2,4))
res <- weighted.median(y, w)</pre>

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