# Package 'fastmatrix'

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Title Fast Computation of some Matrices Useful in Statistics

Type Package

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Description Small set of functions to fast computation of some matrices and operations useful in statistics and econometrics. Currently, there are functions for efficient computation of duplication, commutation and symmetrizer matrices with minimal storage requirements. Some commonly used matrix decompositions (LU and LDL), basic matrix operations (for instance, Hadamard, Kronecker products and the Sherman-Morrison formula) and iterative solvers for linear systems are also available. In addition, the package includes a number of common statistical procedures such as the sweep operator, weighted mean and covariance matrix using an online algorithm, linear regression (using Cholesky, QR, SVD, sweep operator and conjugate gradients methods), ridge regression (with optimal selection of the ridge parameter considering the GCV procedure), functions to compute the multivariate skewness, kurtosis, Mahalanobis distance (checking the positive defineteness) and the Wilson-Hilferty transformation of chi squared variables. Furthermore, the package provides interfaces to C code callable by another C code from other R packages.
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array.mult

Array multiplication

# Description

Multiplication of 3-dimensional arrays was first introduced by Bates and Watts (1980). More extensions and technical details can be found in Wei (1998).

## Usage

```
array.mult(a, b, x)
```

#### Arguments

a numeric matrix.

b a numeric matrix.

x a three-dimensional array.

## **Details**

Let  $X = (x_{tij})$  be a 3-dimensional  $n \times p \times q$  where indices t, i and j indicate face, row and column, respectively. The product Y = AXB is an  $n \times r \times s$  array, with A and B are  $r \times p$  and  $q \times s$  matrices respectively. The elements of Y are defined as:

$$y_{tkl} = \sum_{i=1}^{p} \sum_{j=1}^{q} a_{ki} x_{tij} b_{jl}$$

#### Value

array.mult returns a 3-dimensional array of dimension  $n \times r \times s$ .

# References

Bates, D.M., Watts, D.G. (1980). Relative curvature measures of nonlinearity. *Journal of the Royal Statistical Society, Series B* **42**, 1-25.

Wei, B.C. (1998). Exponential Family Nonlinear Models. Springer, New York.

## See Also

array, matrix, bracket.prod.

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## **Examples**

```
x <- array(0, dim = c(2,3,3)) # 2 x 3 x 3 array
x[,,1] <- c(1,2,2,4,3,6)
x[,,2] <- c(2,4,4,8,6,12)
x[,,3] <- c(3,6,6,12,9,18)

a <- matrix(1, nrow = 2, ncol = 3)
b <- matrix(1, nrow = 3, ncol = 2)

y <- array.mult(a, b, x) # a 2 x 2 x 2 array
y</pre>
```

 ${\it asSymmetric}$ 

Force a matrix to be symmetric

# Description

Force a square matrix x to be symmetric

## Usage

```
asSymmetric(x, lower = TRUE)
```

# Arguments

x a square matrix to be forced to be symmetric.

lower logical, should the upper (lower) triangle be replaced with the lower (upper) triangle?

## Value

a square symmetric matrix.

```
a <- matrix(1:16, ncol = 4)
isSymmetric(a) # FALSE
a <- asSymmetric(a) # copy lower triangle into upper triangle</pre>
```

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bezier

Computation of Bezier curve

#### **Description**

Computes the Bezier curve based on n+1 control points using the De Casteljau's method.

## Usage

```
bezier(x, y, ngrid = 200)
```

# **Arguments**

x, y vector giving the coordinates of the control points. Missing values are deleted.

ngrid number of elements in the grid used to compute the smoother.

#### **Details**

Given  $p_0, p_1, \dots, p_n$  control points the Bezier curve is given by B(t) defined as

$$B(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \sum_{k=0}^{n} \binom{n}{k} t^{k} (1-t)^{k} \boldsymbol{p}_{k}$$

where  $t \in [0, 1]$ . To evaluate the Bezier curve the De Casteljau's method is used.

## Value

A list containing xgrid and ygrid elements used to plot the Bezier curve.

```
# a tiny example
x <- c(1.0, 0.25, 1.25, 2.5, 4.00, 5.0)
y <- c(0.5, 2.00, 3.75, 4.0, 3.25, 1.0)
plot(x, y, type = "o")
z <- bezier(x, y, ngrid = 50)
lines(z$xgrid, z$ygrid, lwd = 2, lty = 2, col = "red")
# other simple example
x <- c(4,6,4,5,6,7)
y <- 1:6
plot(x, y, type = "o")
z <- bezier(x, y, ngrid = 50)
lines(z$xgrid, z$ygrid, lwd = 2, lty = 2, col = "red")</pre>
```

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bracket.prod

Bracket product

## **Description**

Bracket product of a matrix and a 3-dimensional array.

## Usage

```
bracket.prod(a, x)
```

## Arguments

a numeric matrix.

x a three-dimensional array.

#### **Details**

Let  $X = (x_{tij})$  be a 3-dimensional  $n \times p \times q$  array and A an  $m \times n$  matrix, then Y = [A][X] is called the bracket product of A and X, that is an  $m \times p \times q$  with elements

$$y_{tij} = \sum_{k=1}^{n} a_{tk} x_{kij}$$

#### Value

bracket.prod returns a 3-dimensional array of dimension  $m \times p \times q$ .

#### References

Wei, B.C. (1998). Exponential Family Nonlinear Models. Springer, New York.

## See Also

```
array, matrix, array.mult.
```

```
x \leftarrow array(0, dim = c(2,3,3)) \# 2 \times 3 \times 3 array \\ x[,,1] \leftarrow c(1,2,2,4,3,6) \\ x[,,2] \leftarrow c(2,4,4,8,6,12) \\ x[,,3] \leftarrow c(3,6,6,12,9,18) \\ a \leftarrow arrix(1, nrow = 3, ncol = 2) \\ y \leftarrow bracket.prod(a, x) \# a 3 x 3 x 3 array \\ y
```

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cg

Solve linear systems using the conjugate gradients method

# Description

Conjugate gradients (CG) method is an iterative algorithm for solving linear systems with positive definite coefficient matrices.

#### **Usage**

```
cg(a, b, maxiter = 200, tol = 1e-7)
```

## **Arguments**

а	a symmetric positive definite matrix containing the coefficients of the linear system.
b	a vector of right-hand sides of the linear system.
maxiter	the maximum number of iterations. Defaults to 200
tol	tolerance level for stopping iterations.

#### Value

a vector with the approximate solution, the iterations performed are returned as the attribute 'iterations'.

#### Warning

The underlying C code does not check for symmetry nor positive definitiveness.

# References

Golub, G.H., Van Loan, C.F. (1996). *Matrix Computations*, 3rd Edition. John Hopkins University Press.

Hestenes, M.R., Stiefel, E. (1952). Methods of conjugate gradients for solving linear equations. *Journal of Research of the National Bureau of Standards* **49**, 409-436.

## See Also

```
jacobi, seidel, solve
```

```
a <- matrix(c(4,3,0,3,4,-1,0,-1,4), ncol = 3)
b <- c(24,30,-24)
z <- cg(a, b)
z # 3 iterations</pre>
```

8 comm.info

comm.info	Compact information to construct the commutation matrix
Comm. 1111 o	Compact information to construct the communication matrix

## **Description**

This function provides the minimum information required to create the commutation matrix.

The commutation matrix is a square matrix of order mn that, for an  $m \times n$  matrix A, transform vec(A) to  $vec(A^T)$ .

# Usage

```
comm.info(m = 1, n = m, condensed = TRUE)
```

## **Arguments**

m a positive integer row dimension.n a positive integer column dimension.

condensed logical. Information should be returned in compact form?

#### **Details**

This function returns a list containing two vectors that represent an element of the commutation matrix and is accessed by the indexes in vectors row and col. This information is used by function comm.prod to do some operations involving the commutation matrix without forming it. This information also can be obtained using function commutation.

#### Value

A list containing the following elements:

row	vector of indexes, each entry represents the row index of the commutation matrix.
col	vector of indexes, each entry represents the column index of the commutation matrix. Only present if condensed = FALSE.
m	positive integer, row dimension.
n	positive integer, column dimension.

## References

Magnus, J.R., Neudecker, H. (1979). The commutation matrix: some properties and applications. *The Annals of Statistics* **7**, 381-394.

## See Also

```
commutation, comm.prod
```

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## **Examples**

```
z <- comm.info(m = 3, n = 2, condensed = FALSE)
z # where are the ones in commutation matrix of order '3,2'?

K32 <- commutation(m = 3, n = 2, matrix = TRUE)

K32 # only recommended if m and n are very small</pre>
```

comm.prod

Matrix multiplication envolving the commutation matrix

## **Description**

Given the row and column dimension of a commutation and matrix x, performs one of the matrix-matrix operations:

```
ullet Y=KX, if side = "left" and transposed = FALSE, or
```

- $oldsymbol{Y} = oldsymbol{K}^T oldsymbol{X}$ , if side = "left" and transposed = TRUE, or
- Y = XK, if side = "right" and transposed = FALSE, or
- $oldsymbol{Y} = oldsymbol{X} oldsymbol{K}^T,$  if side = "right" and transposed = TRUE,

where K is the commutation matrix of order mn. The main aim of comm. prod is to do this matrix multiplication without forming the commutation matrix.

# Usage

```
comm.prod(m = 1, n = m, x = NULL, transposed = FALSE, side = "left")
```

#### **Arguments**

m a positive integer row dimension.
 n a positive integer column dimension.
 x numeric matrix (or vector).
 transposed logical. Commutation matrix should be transposed?

side a string selecting if commutation matrix is pre-multiplying x, that is side =

"left" or post-multiplying x, by using side = "right".

#### **Details**

Underlying Fortran code only uses information provided by comm.info to performs the matrix multiplication. The commutation matrix is **never** created.

#### See Also

commutation

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## **Examples**

```
K42 <- commutation(m = 4, n = 2, matrix = TRUE) x <- matrix(1:24, ncol = 3) y <- K42 %*% x z <- comm.prod(m = 4, n = 2, x) # K42 is not stored all(z == y) # matrices y and z are equal!
```

commutation

Commutation matrix

#### **Description**

This function returns the commutation matrix of order mn which transforms, for an  $m \times n$  matrix A, vec(A) to  $vec(A^T)$ .

# Usage

```
commutation(m = 1, n = m, matrix = FALSE, condensed = FALSE)
```

## **Arguments**

m a positive integer row dimension.n a positive integer column dimension.

matrix a logical indicating whether the commutation matrix will be returned.

condensed logical. Information should be returned in compact form?

## Details

This function is a wrapper function for the function comm.info. This function provides the minimum information required to create the commutation matrix. If option matrix = FALSE the commutation matrix is stored in two vectors containing the coordinate list of indexes for rows and columns. Option condensed = TRUE only returns vector of indexes for the rows of commutation matrix.

**Warning:** matrix = TRUE is **not** recommended, unless the order m **and** n be small. This matrix can require a huge amount of storage.

#### Value

Returns an mn by mn matrix (if requested).

#### References

Magnus, J.R., Neudecker, H. (1979). The commutation matrix: some properties and applications. *The Annals of Statistics* **7**, 381-394.

Magnus, J.R., Neudecker, H. (2007). *Matrix Differential Calculus with Applications in Statistics and Econometrics*, 3rd Edition. Wiley, New York.

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#### See Also

```
comm.info
```

## **Examples**

```
z <- commutation(m = 100, condensed = TRUE)
object.size(z) # 40.6 Kb of storage

z <- commutation(m = 100, condensed = FALSE)
object.size(z) # 80.7 Kb of storage

K100 <- commutation(m = 100, matrix = TRUE) # time: < 2 secs
object.size(K100) # 400 Mb of storage, do not request this matrix!

# a small example
K32 <- commutation(m = 3, n = 2, matrix = TRUE)
a <- matrix(1:6, ncol = 2)
v <- K32 %*% vec(a)
all(vec(t(a)) == as.vector(v)) # vectors are equal!</pre>
```

cov.MSSD

Mean Square Successive Difference (MSSD) estimator of the covariance matrix

# Description

Returns a list containing the mean and covariance matrix of the data.

#### Usage

```
cov.MSSD(x)
```

# Arguments

Х

a matrix or data frame. As usual, rows are observations and columns are variables.

#### **Details**

This procedure uses the Holmes-Mergen method using the difference between each successive pairs of observations also known as Mean Square Successive Method (MSSD) to estimate the covariance matrix.

#### Value

A list containing the following named components:

mean an estimate for the center (mean) of the data.

cov the estimated covariance matrix.

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#### References

Holmes, D.S., Mergen, A.E. (1993). Improving the performance of the  $T^2$  control chart. *Quality Engineering* 5, 619-625.

#### See Also

```
cov and var.
```

#### **Examples**

```
x <- cbind(1:10, c(1:3, 8:5, 8:10))
z0 <- cov(x)
z0
z1 <- cov.MSSD(x)
z1</pre>
```

cov.weighted

Weighted covariance matrices

# Description

Returns a list containing estimates of the weighted mean and covariance matrix of the data.

#### **Usage**

```
cov.weighted(x, weights = rep(1, nrow(x)))
```

# **Arguments**

x a matrix or data frame. As usual, rows are observations and columns are vari-

ables.

weights a non-negative and non-zero vector of weights for each observation. Its length

must equal the number of rows of x.

#### **Details**

The covariance matrix is divided by the number of observations, which arise for instance, when we use the class of elliptical contoured distributions. This differs from the behaviour of function cov.wt.

#### Value

A list containing the following named components:

mean an estimate for the center (mean) of the data.
cov the estimated (weighted) covariance matrix.

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#### References

Clarke, M.R.B. (1971). Algorithm AS 41: Updating the sample mean and dispersion matrix. *Applied Statistics* **20**, 206-209.

#### See Also

```
cov.wt, cov and var.
```

## **Examples**

```
x <- cbind(1:10, c(1:3, 8:5, 8:10))
z0 <- cov.weighted(x) # all weights are 1
D2 <- Mahalanobis(x, center = z0$mean, cov = z0$cov)
p <- ncol(x)
wts <- (p + 1) / (1 + D2) # nice weights!
z1 <- cov.weighted(x, weights = wts)
z1</pre>
```

dupl.cross

Matrix crossproduct envolving the duplication matrix

## **Description**

Given the order of two duplication matrices and matrix x, this function performs the operation:  $Y = D_n^T X D_k$ , where  $D_n$  and  $D_k$  are duplication matrices of order n and k, respectively.

## Usage

```
dupl.cross(n = 1, k = n, x = NULL)
```

# **Arguments**

- n order of the duplication matrix used pre-multiplying x.
- k order of the duplication matrix used post-multiplying x. By default k = n is used.
- x numeric matrix, this argument is required.

## **Details**

This function calls dupl.prod to performs the matrix multiplications required but **without forming** any duplication matrices.

#### See Also

```
dupl.prod
```

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#### **Examples**

```
D2 <- duplication(n = 2, matrix = TRUE)
D3 <- duplication(n = 3, matrix = TRUE)
x <- matrix(1, nrow = 9, ncol = 4)
y <- t(D3) %*% x %*% D2

z <- dupl.cross(n = 3, k = 2, x) # D2 and D3 are not stored
all(z == y) # matrices y and z are equal!

x <- matrix(1, nrow = 9, ncol = 9)
z <- dupl.cross(n = 3, x = x) # same matrix is used to pre- and post-multiplying x z # print result</pre>
```

dupl.info

Compact information to construct the duplication matrix

## **Description**

This function provides the minimum information required to create the duplication matrix.

#### Usage

```
dupl.info(n = 1, condensed = TRUE)
```

## **Arguments**

n order of the duplication matrix.

condensed logical. Information should be returned in compact form?

## **Details**

This function returns a list containing two vectors that represent an element of the duplication matrix and is accessed by the indexes in vectors row and col. This information is used by function dupl.prod to do some operations involving the duplication matrix without forming it. This information also can be obtained using function duplication

## Value

A list containing the following elements:

row	vector of indexes, each entry represents the row index of the duplication matrix. Only present if condensed = FALSE.
col	vector of indexes, each entry represents the column index of the duplication matrix.
order	order of the duplication matrix.

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#### See Also

```
duplication, dupl.prod
```

## **Examples**

```
z <- dupl.info(n = 3, condensed = FALSE)
z # where are the ones in duplication of order 3?

D3 <- duplication(n = 3, matrix = TRUE)
D3 # only recommended if n is very small</pre>
```

dupl.prod

Matrix multiplication envolving the duplication matrix

# **Description**

Given the order of a duplication and matrix x, performs one of the matrix-matrix operations:

```
ullet Y=DX, if side = "left" and transposed = FALSE, or
```

•  $oldsymbol{Y} = oldsymbol{D}^T oldsymbol{X}, ext{ if side = "left" and transposed = TRUE, or}$ 

ullet  $oldsymbol{Y}=oldsymbol{X}oldsymbol{D},$  if side = "right" and transposed = FALSE, or

•  $oldsymbol{Y} = oldsymbol{X} oldsymbol{D}^T,$  if side = "right" and transposed = TRUE,

where D is the duplication matrix of order n. The main aim of dupl.prod is to do this matrix multiplication without forming the duplication matrix.

#### Usage

```
dupl.prod(n = 1, x, transposed = FALSE, side = "left")
```

## **Arguments**

n order of the duplication matrix.
x numeric matrix (or vector).

transposed logical. Duplication matrix should be transposed?

side a string selecting if duplication matrix is pre-multiplying x, that is side = "left"

or post-multiplying x, by using side = "right".

## **Details**

Underlying C code only uses information provided by dupl.info to performs the matrix multiplication. The duplication matrix is **never** created.

## See Also

```
duplication
```

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## **Examples**

```
D4 <- duplication(n = 4, matrix = TRUE)
x <- matrix(1, nrow = 16, ncol = 2)
y <- crossprod(D4, x)

z <- dupl.prod(n = 4, x, transposed = TRUE) # D4 is not stored
all(z == y) # matrices y and z are equal!</pre>
```

duplication

Duplication matrix

## Description

This function returns the duplication matrix of order n which transforms, for a symmetric matrix A, vech(A) into vec(A).

#### Usage

```
duplication(n = 1, matrix = FALSE, condensed = FALSE)
```

# **Arguments**

n order of the duplication matrix.

matrix a logical indicating whether the duplication matrix will be returned.

condensed logical. Information should be returned in compact form?.

#### **Details**

This function is a wrapper function for the function dupl.info. This function provides the minimum information required to create the duplication matrix. If option matrix = FALSE the duplication matrix is stored in two vectors containing the coordinate list of indexes for rows and columns. Option condensed = TRUE only returns vector of indexes for the columns of duplication matrix.

**Warning:** matrix = TRUE is **not** recommended, unless the order n be small. This matrix can require a huge amount of storage.

#### Value

Returns an  $n^2$  by n(n+1)/2 matrix (if requested).

#### References

Magnus, J.R., Neudecker, H. (1980). The elimination matrix, some lemmas and applications. *SIAM Journal on Algebraic Discrete Methods* **1**, 422-449.

Magnus, J.R., Neudecker, H. (2007). *Matrix Differential Calculus with Applications in Statistics and Econometrics*, 3rd Edition. Wiley, New York.

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## See Also

```
dupl.info
```

# **Examples**

equilibrate

Equilibration of a rectangular or symmetric matrix

## **Description**

Equilibrate a rectangular or symmetric matrix using 2-norm.

# Usage

```
equilibrate(x, scale = TRUE)
```

# Arguments

```
x a numeric matrix.
scale a logical value, x must be scaled to norm unity?
```

## Value

For scale = TRUE, the equilibrated matrix. The scalings and an approximation of the condition number, are returned as attributes "scales" and "condition". If x is a rectangular matrix, only the columns are equilibrated.

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#### **Examples**

geomean

Geometric mean

## **Description**

It calculates the geometric mean using a Fused-Multiply-and-Add (FMA) compensated scheme for accurate computation of floating-point product.

#### Usage

```
geomean(x)
```

## **Arguments**

Х

a numeric vector containing the sample observations.

## **Details**

If x contains any non-positive values, geomean returns NA and a warning message is displayed.

The geometric mean is a measure of central tendency, which is defined as

$$G = \sqrt[n]{x_1 x_2 \dots x_n} = \left(\prod_{i=1}^n x_i\right)^{1/n}.$$

This procedure calculates the product required in the geometric mean safely using a compensated scheme as proposed by Graillat (2009).

#### Value

The geometric mean of the sample, a non-negative number.

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#### References

Graillat, S. (2009). Accurate floating-point product and exponentiation. *IEEE Transactions on Computers* **58**, 994-1000.

Oguita, T., Rump, S.M., Oishi, S. (2005). Accurate sum and dot product. *SIAM Journal on Scientific Computing* **26**, 1955-1988.

#### See Also

```
mean, median.
```

# **Examples**

```
set.seed(149)
x <- rlnorm(1000)
mean(x) # 1.68169
median(x) # 0.99663
geomean(x) # 1.01688</pre>
```

hadamard

Hadamard product of two matrices

## **Description**

This function returns the Hadamard or element-wise product of two matrices x and y, that have the same dimensions.

## Usage

```
hadamard(x, y = x)
```

# Arguments

```
x a numeric matrix or vector.
y a numeric matrix or vector.
```

## Value

A matrix with the same dimension of x (and y) which corresponds to the element-by-element product of the two matrices.

## References

Styan, G.P.H. (1973). Hadamard products and multivariate statistical analysis, *Linear Algebra and Its Applications* **6**, 217-240.

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## **Examples**

```
x <- matrix(rep(1:10, times = 5), ncol = 5)
y <- matrix(rep(1:5, each = 10), ncol = 5)
z <- hadamard(x, y)
z</pre>
```

helmert

Helmert matrix

# Description

This function returns the Helmert matrix of order n.

## Usage

```
helmert(n = 1)
```

#### Arguments

n

order of the Helmert matrix.

## **Details**

A Helmert matrix of order n is a square matrix defined as

$$\boldsymbol{H}_{n} = \begin{bmatrix} 1/\sqrt{n} & 1/\sqrt{n} & 1/\sqrt{n} & \dots & 1/\sqrt{n} \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 & \dots & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \dots & -\frac{(n-1)}{\sqrt{n(n-1)}} \end{bmatrix}.$$

Helmert matrix is orthogonal and is frequently used in the analysis of variance (ANOVA).

#### Value

Returns an n by n matrix.

# References

Lancaster, H.O. (1965). The Helmert matrices. *The American Mathematical Monthly* **72**, 4-12. Gentle, J.E. (2007). *Matrix Algebra: Theory, Computations, and Applications in Statistics*. Springer, New York.

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## **Examples**

```
n <- 1000
set.seed(149)
x <- rnorm(n)

H <- helmert(n)
object.size(H) # 7.63 Mb of storage
K <- H[2:n,]
z <- c(K %*% x)
sum(z^2) # 933.1736

# same that
(n - 1) * var(x)</pre>
```

is.lower.tri

Check if a matrix is lower or upper triangular

# Description

Returns TRUE if the given matrix is lower or upper triangular matrix.

## Usage

```
is.lower.tri(x, diag = FALSE)
is.upper.tri(x, diag = FALSE)
```

# Arguments

```
x a matrix of other R object with length(dim(x)) == 2.
diag logical. Should the diagonal be included?
```

## Value

Check if a matrix is lower or upper triangular. You can also include diagonal to the check.

## See Also

```
lower.tri, upper.tri
```

```
x <- matrix(rnorm(10 * 3), ncol = 3)
R <- chol(crossprod(x))
is.lower.tri(R)
is.upper.tri(R)</pre>
```

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jacobi

Solve linear systems using the Jacobi method

#### **Description**

Jacobi method is an iterative algorithm for solving a system of linear equations.

#### Usage

```
jacobi(a, b, start, maxiter = 200, tol = 1e-7)
```

#### **Arguments**

a a square numeric matrix containing the coefficients of the linear system.

b a vector of right-hand sides of the linear system.

start a vector for initial starting point.

maxiter the maximum number of iterations. Defaults to 200

tol tolerance level for stopping iterations.

#### **Details**

Let D, L, and U denote the diagonal, lower triangular and upper triangular parts of a matrix A. Jacobi's method solve the equation Ax = b, iteratively by rewriting Dx + (L + U)x = b. Assuming that D is nonsingular leads to the iteration formula

$$\boldsymbol{x}^{(k+1)} = -\boldsymbol{D}^{-1}(\boldsymbol{L} + \boldsymbol{U})\boldsymbol{x}^{(k)} + \boldsymbol{D}^{-1}\boldsymbol{b}$$

#### Value

a vector with the approximate solution, the iterations performed are returned as the attribute 'iterations'.

# References

Golub, G.H., Van Loan, C.F. (1996). *Matrix Computations*, 3rd Edition. John Hopkins University Press.

## See Also

seidel

```
a <- matrix(c(5,-3,2,-2,9,-1,3,1,-7), ncol = 3)
b <- c(-1,2,3)
start <- c(1,1,1)
z <- jacobi(a, b, start)
z # 15 iterations
```

kronecker.prod 23

kronecker.prod

Kronecker product on matrices

## Description

Computes the kronecker product of two matrices, x and y.

# Usage

```
kronecker.prod(x, y = x)
```

## **Arguments**

x a numeric matrix or vector.

y a numeric matrix or vector.

#### **Details**

Let  $\boldsymbol{X}$  be an  $m \times n$  and  $\boldsymbol{Y}$  a  $p \times q$  matrix. The  $mp \times nq$  matrix defined by

$$\left[\begin{array}{ccc} x_{11}Y & \dots & x_{1n}Y \\ \vdots & & \vdots \\ x_{m1}Y & \dots & x_{mn}Y \end{array}\right],$$

is called the  $Kronecker\ product$  of X and Y.

# Value

An array with dimensions dim(x) \* dim(y).

## References

Magnus, J.R., Neudecker, H. (2007). *Matrix Differential Calculus with Applications in Statistics and Econometrics*, 3rd Edition. Wiley, New York.

#### See Also

kronecker function from base package is based on outer. Our C version is slightly faster.

```
# block diagonal matrix:
a <- diag(1:3)
b <- matrix(1:4, ncol = 2)
kronecker.prod(a, b)

# examples with vectors
ones <- rep(1, 4)</pre>
```

24 kurtosis

```
y <- 1:3
kronecker.prod(ones, y) # 12-dimensional vector
kronecker.prod(ones, t(y)) # 3 x 3 matrix</pre>
```

kurtosis

Mardia's multivariate skewness and kurtosis coefficients

#### **Description**

Functions to compute measures of multivariate skewness  $(b_{1p})$  and kurtosis  $(b_{2p})$  proposed by Mardia (1970),

$$b_{1p} = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n ((\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{S}^{-1} (\boldsymbol{x}_j - \overline{\boldsymbol{x}}))^3,$$

and

$$b_{2p} = \frac{1}{n} \sum_{i=1}^{n} ((\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{S}^{-1} (\boldsymbol{x}_j - \overline{\boldsymbol{x}}))^2.$$

#### Usage

kurtosis(x)

skewness(x)

#### **Arguments**

Χ

matrix of data with, say, p columns.

## References

Mardia, K.V. (1970). Measures of multivariate skewness and kurtosis with applications. *Biometrika* **57**, 519-530.

Mardia, K.V., Zemroch, P.J. (1975). Algorithm AS 84: Measures of multivariate skewness and kurtosis. *Applied Statistics* **24**, 262-265.

```
setosa <- iris[1:50,1:4]
kurtosis(setosa)
skewness(setosa)</pre>
```

ldl 25

ldl

The LDL decomposition

## Description

Compute the LDL decomposition of a real symmetric matrix.

# Usage

ldl(x)

## **Arguments**

Х

a symmetric numeric matrix whose LDL decomposition is to be computed.

#### Value

The factorization has the form  $X = LDL^T$ , where D is a diagonal matrix and L is unitary lower triangular.

The LDL decomposition of x is returned as a list with components:

lower the unitary lower triangular factor L.

d a vector containing the diagonal elements of D.

#### References

Golub, G.H., Van Loan, C.F. (1996). *Matrix Computations*, 3rd Edition. John Hopkins University Press.

## See Also

chol

```
a <- matrix(c(2,-1,0,-1,2,-1,0,-1,1), ncol = 3)
z <- ldl(a)
z # information of LDL factorization

# computing det(a)
prod(z$d) # product of diagonal elements of D

# a non-positive-definite matrix
m <- matrix(c(5,-5,-5,3), ncol = 2)
try(chol(m)) # fails
ldl(m)</pre>
```

26 lu

lu

The LU factorization of a square matrix

## Description

lu computes the LU factorization of a matrix.

# Usage

```
lu(x)
## Default S3 method:
lu(x)
## S3 method for class 'lu'
solve(a, b, ...)
is.lu(x)
```

## **Arguments**

x a square numeric matrix whose LU factorization is to be computed.

a an LU factorization of a square matrix.

b a vector or matrix of right-hand sides of equations.

... further arguments passed to or from other methods

#### **Details**

The LU factorization plays an important role in many numerical procedures. In particular it is the basic method to solve the equation Ax = b for given matrix A, and vector b.

```
solve.lu is the method for solve for lu objects.
```

```
is.lu returns TRUE if x is a list and inherits from "lu".
```

Unsuccessful results from the underlying LAPACK code will result in an error giving a positive error code: these can only be interpreted by detailed study of the Fortran code.

## Value

The LU factorization of the matrix as computed by LAPACK. The components in the returned value correspond directly to the values returned by DGETRF.

1u a matrix with the same dimensions as x. The upper triangle contains the U of

the decomposition and the strict lower triangle contains information on the  $m{L}$  of

the factorization.

pivot information on the pivoting strategy used during the factorization.

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#### Note

To compute the determinant of a matrix (do you *really* need it?), the LU factorization is much more efficient than using eigenvalues (eigen). See det.

LAPACK uses column pivoting and does not attempt to detect rank-deficient matrices.

#### References

Anderson. E., Bai, Z., Bischof, C., Blackford, S., Demmel, J., Dongarra, J., Du Croz, J., Greenbaum, A., Hammarling, S., McKenney, A. Sorensen, D. (1999). *LAPACK Users' Guide*, 3rd Edition. SIAM. (Available at http://www.netlib.org/lapack/lug/lapack\_lug.html).

Golub, G.H., Van Loan, C.F. (1996). *Matrix Computations*, 3rd Edition. John Hopkins University Press.

#### See Also

extractL, extractU, constructX for reconstruction of the matrices, lu2inv

## **Examples**

```
a <- matrix(c(3,2,6,17,4,18,10,-2,-12), ncol = 3)
z <- lu(a)
z # information of LU factorization

# computing det(a)
prod(diag(z$lu)) # product of diagonal elements of U

# solve linear equations
b <- matrix(1:6, ncol = 2)
solve(z, b)</pre>
```

lu-methods

Reconstruct the L, U, or X Matrices from an LU object

# Description

Returns the original matrix from which the object was constructed or the components of the factorization.

## Usage

```
constructX(x)
extractL(x)
extractU(x)
```

#### **Arguments**

x object representing an LU factorization. This will typically have come from a previous call to lu.

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#### Value

construct X returns X, the original matrix from which the lu object was constructed (because of the pivoting the X matrix is not exactly the product between L and U).

```
extractL returns oldsymbol{L}. This may be pivoted.
```

extractU returns  $oldsymbol{U}$ .

#### See Also

lu.

#### **Examples**

```
a <- matrix(c(10,-3,5,-7,2,-1,0,6,5), ncol = 3)
z <- lu(a)
L <- extractL(z)
L
U <- extractU(z)
U
X <- constructX(z)
all(a == X)</pre>
```

lu2inv

 ${\it Inverse from LU factorization}$ 

## **Description**

Invert a square matrix from its LU factorization.

#### Usage

```
lu2inv(x)
```

# Arguments

Х

object representing an LU factorization. This will typically have come from a previous call to lu.

#### Value

The inverse of the matrix whose LU factorization was given.

Unsuccessful results from the underlying LAPACK code will result in an error giving a positive error code: these can only be interpreted by detailed study of the Fortran code.

#### **Source**

This is an interface to the LAPACK routine DGETRI. LAPACK is from <a href="https://www.netlib.org/lapack/">https://www.netlib.org/lapack/</a> and its guide is listed in the references.

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#### References

Anderson. E., Bai, Z., Bischof, C., Blackford, S., Demmel, J., Dongarra, J., Du Croz, J., Greenbaum, A., Hammarling, S., McKenney, A. Sorensen, D. (1999). *LAPACK Users' Guide*, 3rd Edition. SIAM. (Available at http://www.netlib.org/lapack/lug/lapack\_lug.html).

Golub, G.H., Van Loan, C.F. (1996). *Matrix Computations*, 3rd Edition. John Hopkins University Press.

#### See Also

lu, solve.

## **Examples**

```
a <- matrix(c(3,2,6,17,4,18,10,-2,-12), ncol = 3)
z <- lu(a)
a %*% lu2inv(z)</pre>
```

Mahalanobis

Mahalanobis distance

## **Description**

Returns the squared Mahalanobis distance of all rows in x and the vector  $\mu$  = center with respect to  $\Sigma$  = cov. This is (for vector x) defined as

$$D^2 = (\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})$$

#### Usage

Mahalanobis(x, center, cov, inverted = FALSE)

# **Arguments**

x vector or matrix of data. As usual, rows are observations and columns are vari-

ables.

center mean vector of the distribution.

cov covariance matrix  $(p \times p)$  of the distribution, must be positive definite.

inverted logical. If TRUE, cov is supposed to contain the *inverse* of the covariance matrix.

#### **Details**

Unlike function mahalanobis, the covariance matrix is factorized using the Cholesky decomposition, which allows to assess if cov is positive definite. Unsuccessful results from the underlying LAPACK code will result in an error message.

## See Also

cov, mahalanobis

30 matrix.inner

## **Examples**

```
x <- cbind(1:6, 1:3)
xbar <- colMeans(x)
S <- matrix(c(1,4,4,1), ncol = 2) # is negative definite
D2 <- mahalanobis(x, center = xbar, S)
all(D2 >= 0) # several distances are negative
## next command produces the following error:
## Covariance matrix is possibly not positive-definite
## Not run: D2 <- Mahalanobis(x, center = xbar, S)</pre>
```

matrix.inner

Compute the inner product between two rectangular matrices

## **Description**

Computes the inner product between two rectangular matrices calling BLAS.

# Usage

```
matrix.inner(x, y = x)
```

## **Arguments**

```
x a numeric matrix.
y a numeric matrix.
```

## Value

a real value, indicating the inner product between two matrices.

matrix.norm 31

matrix.norm

Compute the norm of a rectangular matrix

## **Description**

Computes a matrix norm of x using LAPACK. The norm can be the one ("1") norm, the infinity ("inf") norm, the Frobenius norm, the maximum modulus ("maximum") among elements of a matrix, as determined by the value of type.

## Usage

```
matrix.norm(x, type = "Frobenius")
```

#### **Arguments**

x a numeric matrix.

type character string, specifying the *type* of matrix norm to be computed. A character indicating the type of norm desired.

indicating the type of norm desired.

"1" specifies the **one** norm, (maximum absolute column sum);
"Inf" specifies the **inf**inity norm (maximum absolute row sum);

"Frobenius" specifies the **Frobenius** norm (the Euclidean norm of x treated as if it were a vector);

"maximum" specifies the **maximum** modulus of all the elements in x.

#### Details

As function norm in package **base**, method of matrix.norm calls the LAPACK function DLANGE. Note that the 1-, Inf- and maximum norm is faster to calculate than the Frobenius one.

#### Value

The matrix norm, a non-negative number.

32 mediancenter

```
n <- 1000
x <- .5 * diag(n) + 0.5 * matrix(1, nrow = n, ncol = n)
matrix.norm(x, type = "Frobenius")
matrix.norm(x, type = "1")
matrix.norm(x, type = "Inf")
matrix.norm(x, type = "maximum") # equal to 1</pre>
```

mediancenter

Mediancenter

# Description

It calculates the mediancenter (or geometric median) of multivariate data.

#### Usage

```
mediancenter(x)
```

#### **Arguments**

Χ

a matrix or data frame. As usual, rows are observations and columns are variables.

## **Details**

The mediancenter for a sample of multivariate observations is computed using a steepest descend method combined with bisection. The mediancenter invariant to rotations of axes and is useful as a multivariate generalization of the median of univariate sample.

## Value

A list containing the following named components:

median an estimate for the mediancenter of the data.

iter the number of iterations performed, it is negative if a degenerate solution is

found.

# References

Gower, J.C. (1974). Algorithm AS 78: The mediancentre. Applied Statistics 23, 466-470.

#### See Also

```
cov.wt, median.
```

minkowski 33

#### **Examples**

```
x <- cbind(1:10, c(1:3, 8:5, 8:10))
z <- mediancenter(x)$median # degenerate solution
xbar <- colMeans(x)
plot(x, xlab = "", ylab = "")
points(x = xbar[1], y = xbar[2], pch = 16, col = "red")
points(x = z[1], y = z[2], pch = 3, col = "blue", lwd = 2)</pre>
```

minkowski

Computes the p-norm of a vector

# Description

Computes a p-norm of vector x. The norm can be the one (p = 1) norm, Euclidean (p = 2) norm, the infinity (p = Inf) norm. The underlying C or Fortran code is inspired on ideas of BLAS Level 1.

# Usage

```
minkowski(x, p = 2)
```

## **Arguments**

x a numeric vector.

p a number, specifying the *type* of norm desired. Possible values include real number greater or equal to 1, or Inf, Default value is p = 2.

#### **Details**

Method of minkowski for p = Inf calls idamax BLAS function. For other values, C or Fortran subroutines using unrolled cycles are called.

## Value

The vector p-norm, a non-negative number.

```
# a tiny example
x <- rnorm(1000)
minkowski(x, p = 1)
minkowski(x, p = 1.5)
minkowski(x, p = 2)
minkowski(x, p = Inf)

x <- x / minkowski(x)
minkowski(x, p = 2) # equal to 1</pre>
```

34 moments

moments

Central moments

## **Description**

It calculates up to fourth central moments (or moments about the mean), and the skewness and kurtosis coefficients using an online algorithm.

## Usage

moments(x)

#### **Arguments**

Х

a numeric vector containing the sample observations.

#### **Details**

The k-th central moment is defined as

$$m_k = \frac{1}{n} \sum_{i=1}^n (x_i - \overline{x})^k.$$

In particular, the second central moment is the variance of the sample. The sample skewness and kurtosis are defined, respectively, as

$$b_1 = \frac{m_3}{s^3}, \qquad b_2 = \frac{m_4}{s^4} - 3,$$

where s denotes de standard deviation.

#### Value

A list containing second, third and fourth central moments, and skewness and kurtosis coefficients.

#### References

Spicer, C.C. (1972). Algorithm AS 52: Calculation of power sums of deviations about the mean. *Applied Statistics* **21**, 226-227.

#### See Also

var.

```
set.seed(149)
x <- rnorm(1000)
z <- moments(x)
z</pre>
```

ols 35

ols	Fit linear regression model

## **Description**

Returns an object of class "ols" that represents a linear model fit.

## Usage

```
ols(formula, data, subset, na.action, method = "qr", tol = 1e-7, maxiter = 100,
  model = FALSE, x = FALSE, y = FALSE, contrasts = NULL, ...)
```

## **Arguments**

formula	an object of class "formula" (or one that can be coerced to that class): a symbolic description of the model to be fitted.
data	an optional data frame, list or environment (or object coercible by as.data.frame to a data frame) containing the variables in the model. If not found in data, the variables are taken from environment (formula), typically the environment from which ols is called.
subset	an optional vector specifying a subset of observations to be used in the fitting process.
na.action	a function which indicates what should happen when the data contain NAs. The default is set by the na.action setting of options, and is na.fail if that is unset.
method	the least squares fitting method to be used; the options are "cg" (conjugate gradients), "chol", "qr" (the default), "svd" and "sweep".
tol	tolerance for the conjugate gradients (gc) method. Default is tol = 1e-7.
maxiter	The maximum number of iterations for the conjugate gradients (gc) method. Defaults to 100.
model, x, y	logicals. If TRUE the corresponding components of the fit (the model frame, the model matrix, the response) are returned.
contrasts	an optional list. See the contrasts.arg of model.matrix.default.
	additional arguments (currently disregarded).

## Value

ols returns an object of class "ols".

The function summary is used to obtain and print a summary of the results. The generic accessor functions coefficients, fitted.values and residuals extract various useful features of the value returned by ols.

An object of class "ols" is a list containing at least the following components:

```
coefficients a named vector of coefficients
```

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```
residuals
                    the residuals, that is response minus fitted values.
fitted.values
                   the fitted mean values.
RSS
                   the residual sum of squares.
                   a p \times p matrix of (unscaled) covariances of the \hat{\beta}_j, j = 1, \dots, p.
cov.unscaled
call
                   the matched call.
                    the terms object used.
terms
                    (only where relevant) the contrasts used.
contrasts
                   if requested, the response used.
                   if requested, the model matrix used.
Χ
mode1
                   if requested (the default), the model frame used.
```

## See Also

```
ols.fit, lm, lsfit
```

#### **Examples**

ols.fit

Fitter Functions for Linear Models

#### **Description**

This function is a *switcher* among various numerical fitting functions (ols.fit.cg, ols.fit.chol, ols.fit.qr, ols.fit.svd and ols.fit.sweep). The argument method does the switching: "qr" for ols.fit.qr, etc. This should usually *not* be used directly unless by experienced users.

# Usage

```
ols.fit(x, y, method = "qr", tol = 1e-7, maxiter = 100)
```

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# Arguments

x design matrix of dimension  $n \times q$ . y vector of observations of length n. method currently, methods "cg", "chol", "qr" (default), "svd" and "sweep" are supported. tol tolerance for the conjugate gradients (gc) method. Default is tol = 1e-7. maxiter The maximum number of iterations for the conjugate gradients (gc) method. Defaults to 100.

# Value

# a list with components:

coefficients a named vector of coefficients residuals the residuals, that is response minus fitted values. fitted.values the fitted mean values. RSS the residual sum of squares. cov.unscaled a  $p \times p$  matrix of (unscaled) covariances of the  $\hat{\beta}_i$ ,  $j=1,\ldots,p$ .

# See Also

```
ols.fit.cg, ols.fit.chol, ols.fit.qr, ols.fit.svd, ols.fit.sweep.
```

# **Examples**

```
set.seed(151)
n <- 100
p <- 2
x <- matrix(rnorm(n * p), n, p) # no intercept!
y <- rnorm(n)
fm <- ols.fit(x = x, y = y, method = "chol")
fm</pre>
```

ols.fit-methods

Fit a Linear Model

# **Description**

Fits a linear model, returning the bare minimum computations.

# Usage

```
ols.fit.cg(x, y, tol = 1e-7, maxiter = 100)
ols.fit.chol(x, y)
ols.fit.qr(x, y)
ols.fit.svd(x, y)
ols.fit.sweep(x, y)
```

38 power.method

# **Arguments**

x, y	numeric vectors or matrices for the predictors and the response in a linear model. Typically, but not necessarily, x will be constructed by one of the fitting functions.
tol	tolerance for the conjugate gradients (gc) method. Default is tol = 1e-7.
maxiter	The maximum number of iterations for the conjugate gradients (gc) method. Defaults to 100.

## Value

The bare bones of an ols object: the coefficients, residuals, fitted values, and some information used by summary.ols.

## See Also

```
ols, ols.fit, lm
```

# **Examples**

```
set.seed(151)
n <- 100
p <- 2
x <- matrix(rnorm(n * p), n, p) # no intercept!
y <- rnorm(n)
z <- ols.fit.chol(x, y)
z</pre>
```

power.method

Power method to approximate dominant eigenvalue and eigenvector

# Description

The power method seeks to determine the eigenvalue of maximum modulus, and a corresponding eigenvector.

# Usage

```
power.method(x, only.value = FALSE, maxiter = 100, tol = 1e-8)
```

# **Arguments**

x a symmetric matrix.

only.value if TRUE, only the dominant eigenvalue is returned, otherwise both dominant

eigenvalue and eigenvector are returned.

maxiter the maximum number of iterations. Defaults to 100

tol a numeric tolerance.

ridge 39

# Value

When only value is not true, as by default, the result is a list with components "value" and "vector". Otherwise only the dominan eigenvalue is returned. The performed number of iterations to reach convergence is returned as attribute "iterations".

## See Also

eigen for eigenvalues and eigenvectors computation.

# **Examples**

```
n <- 1000

x <- .5 * diag(n) + 0.5 * matrix(1, nrow = n, ncol = n)

# dominant eigenvalue must be (n + 1) / 2

z <- power.method(x, only.value = TRUE)
```

ridge

Ridge regression

# **Description**

Fit a linear model by ridge regression, returning an object of class "ridge".

# Usage

```
ridge(formula, data, subset, lambda = 1.0, method = "GCV", ngrid = 200, tol = 1e-07,
na.action, model = FALSE, x = FALSE, y = FALSE, contrasts = NULL, ...)
```

# **Arguments**

formula	an object of class "formula" (or one that can be coerced to that class): a symbolic description of the model to be fitted.
data	an optional data frame, list or environment (or object coercible by as.data.frame to a data frame) containing the variables in the model. If not found in data, the variables are taken from environment(formula), typically the environment from which ridge is called.
subset	an optional vector specifying a subset of observations to be used in the fitting process.
na.action	a function which indicates what should happen when the data contain NAs. The default is set by the na.action setting of options, and is na.fail if that is unset.
lambda	a scalar or vector of ridge constants. A value of 0 corresponds to ordinary least squares.

40 ridge

method the method for choosing the ridge parameter lambda. If method = "none", then

lambda is 'fixed'. If method = "GCV" (the default) then the ridge parameter is chosen automatically using the generalized cross validation (GCV) criterion. For method = "grid", optimal value of lambda is selected computing the GCV

criterion over a grid.

ngrid number of elements in the grid used to compute the GCV criterion. Only re-

quired if method = "grid" and lambda is a scalar.

tol tolerance for the optimization of the GCV criterion. Default is 1e-7.

model, x, y logicals. If TRUE the corresponding components of the fit (the model frame, the

model matrix, the response) are returned.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

.. additional arguments to be passed to the low level regression fitting functions

(not implemented).

#### **Details**

ridge function fits in linear ridge regression **without** scaling or centering the regressors and the response. In addition, If an intercept is present in the model, its coefficient is penalized.)

## Value

A list with the following components:

dims dimensions of model matrix.

coefficients a named vector of coefficients.

scale a named vector of coefficients.

fitted.values the fitted mean values.

residuals the residuals, that is response minus fitted values.

RSS the residual sum of squares.

edf the effective number of parameters.

GCV vector (if method = "grid") of GCV values.

HKB HKB estimate of the ridge constant.

LW LW estimate of the ridge constant.

lambda vector (if method = "grid") of lambda values.

optimal value of lambda with the minimum GCV (only relevant if method = "grid").

the matched call.

terms the terms object used.

contrasts (only where relevant) the contrasts used.

y if requested, the response used.

x if requested, the model matrix used.

model if requested, the model frame used.

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#### References

Golub, G.H., Heath, M., Wahba, G. (1979). Generalized cross-validation as a method for choosing a good ridge parameter. *Technometrics* **21**, 215-223.

Hoerl, A.E., Kennard, R.W., Baldwin, K.F. (1975). Ridge regression: Some simulations. *Communication in Statistics* **4**, 105-123.

Hoerl, A.E., Kennard, R.W. (1970). Ridge regression: Biased estimation of nonorthogonal problems. *Technometrics* **12**, 55-67.

Lawless, J.F., Wang, P. (1976). A simulation study of ridge and other regression estimators. *Communications in Statistics* **5**, 307-323.

#### See Also

1m, ols

# **Examples**

```
z <- ridge(GNP.deflator ~ ., data = longley, lambda = 4, method = "grid")
z # ridge regression on a grid over seq(0, 4, length = 200)
z <- ridge(GNP.deflator ~ ., data = longley)
z # ridge parameter selected using GCV (default)</pre>
```

seidel

Solve linear systems using the Gauss-Seidel method

# Description

Gauss-Seidel method is an iterative algorithm for solving a system of linear equations.

# Usage

```
seidel(a, b, start, maxiter = 200, tol = 1e-7)
```

#### **Arguments**

a a square numeric matrix containing the coefficients of the linear system.

b a vector of right-hand sides of the linear system.

start a vector for initial starting point.

maxiter the maximum number of iterations. Defaults to 200

tol tolerance level for stopping iterations.

#### **Details**

Let D, L, and U denote the diagonal, lower triangular and upper triangular parts of a matrix A. Gauss-Seidel method solve the equation Ax = b, iteratively by rewriting (L + D)x + Ux = b. Assuming that L + D is nonsingular leads to the iteration formula

$$x^{(k+1)} = -(L + D)^{-1}Ux^{(k)} + (L + D)^{-1}b$$

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## Value

a vector with the approximate solution, the iterations performed are returned as the attribute 'iterations'.

# References

Golub, G.H., Van Loan, C.F. (1996). *Matrix Computations*, 3rd Edition. John Hopkins University Press.

## See Also

jacobi

# **Examples**

```
a <- matrix(c(5,-3,2,-2,9,-1,3,1,-7), ncol = 3)
b <- c(-1,2,3)
start <- c(1,1,1)
z <- seidel(a, b, start)
z # 10 iterations</pre>
```

sherman.morrison

Sherman-Morrison formula

# **Description**

The Sherman-Morrison formula gives a convenient expression for the inverse of the rank 1 update  $(A + bd^T)$  where A is a  $n \times n$  matrix and b, d are n-dimensional vectors. Thus

$$(A + bd^{T})^{-1} = A^{-1} - \frac{A^{-1}bd^{T}A^{-1}}{1 + d^{T}A^{-1}b}.$$

# Usage

```
sherman.morrison(a, b, d = b, inverted = FALSE)
```

# Arguments

a a numeric matrix.b a numeric vector.d a numeric vector.

inverted logical. If TRUE, a is supposed to contain its *inverse*.

### **Details**

Method of sherman.morrison calls BLAS level 2 subroutines DGEMV and DGER for computational efficiency.

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# Value

a square matrix of the same order as a.

# **Examples**

```
n <- 10
ones <- rep(1, n)
a <- 0.5 * diag(n)
z <- sherman.morrison(a, ones, 0.5 * ones)
7</pre>
```

sweep.operator

Gauss-Jordan sweep operator for symmetric matrices

# **Description**

Perform the sweep operation (or reverse sweep) on the diagonal elements of a symmetric matrix.

## Usage

```
sweep.operator(x, k = 1, reverse = FALSE)
```

# **Arguments**

x a symmetric matrix.

k elements (if k is vector) of the diagonal which will be sweeped.

reverse logical. If reverse = TRUE the reverse sweep is performed.

# **Details**

The symmetric sweep operator is a powerful tool in computational statistics with uses in stepwise regression, conditional multivariate normal distributions, MANOVA, and more.

# Value

a square matrix of the same order as x.

# References

Goodnight, J.H. (1979). A tutorial on the SWEEP operator. The American Statistician 33, 149-158.

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## **Examples**

symm.info

Compact information to construct the symmetrizer matrix

# **Description**

This function provides the information required to create the symmetrizer matrix.

# Usage

```
symm.info(n = 1)
```

#### **Arguments**

n

order of the symmetrizer matrix.

#### **Details**

This function returns a list containing vectors that represent an element of the symmetrizer matrix and is accessed by the indexes in vectors row, col and values contained in val. This information is used by function symm.prod to do some operations involving the symmetrizer matrix without forming it. This information also can be obtained using function symmetrizer.

#### Value

A list containing the following elements:

row	vector of indexes, each entry represents the row index of the symmetrizer matrix.
col	vector of indexes, each entry represents the column index of the symmetrizer matrix.
val	vector of values, each entry represents the value of the symmetrizer matrix at element given by row and col indexes.
order	order of the symmetrizer matrix.

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# See Also

```
symmetrizer, symm.prod
```

## **Examples**

```
z <- symm.info(n = 3)
z # elements in symmetrizer matrix of order 3
N3 <- symmetrizer(n = 3, matrix = TRUE)
N3 # only recommended if n is very small</pre>
```

symm.prod

Matrix multiplication envolving the symmetrizer matrix

# Description

Given the order of a symmetrizer and matrix x, performs one of the matrix-matrix operations:

```
    Y = NX, if side = "left", or
    Y = XN, if side = "right",
```

where N is the symmetrizer matrix of order n. The main aim of symm.prod is to do this matrix multiplication without forming the symmetrizer matrix.

## Usage

```
symm.prod(n = 1, x = NULL, side = "left")
```

## **Arguments**

n order of the symmetrizer matrix.

x numeric matrix (or vector).

side a string selecting if symmetrizer matrix is pre-multiplying x, that is side = "left" or post-multiplying x, by using side = "right".

## **Details**

Underlying C code only uses information provided by symm.info to performs the matrix multiplication. The symmetrizer matrix is **never** created.

#### See Also

```
symmetrizer
```

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# **Examples**

```
N4 <- symmetrizer(n = 4, matrix = TRUE)
x <- matrix(1:32, ncol = 2)
y <- N4 %*% x

z <- symm.prod(n = 4, x) # N4 is not stored
all(z == y) # matrices y and z are equal!</pre>
```

symmetrizer

Symmetrizer matrix

# **Description**

This function returns the symmetrizer matrix of order n which transforms, for every  $n \times n$  matrix A, vec(A) into  $vec((A + A^T)/2)$ .

# Usage

```
symmetrizer(n = 1, matrix = FALSE)
```

# **Arguments**

n order of the symmetrizer matrix.

matrix a logical indicating whether the symmetrizer matrix will be returned.

# Details

This function is a wrapper function for the function symm.info. This function provides the information required to create the symmetrizer matrix. If option matrix = FALSE the symmetrizer matrix is stored in three vectors containing the coordinate list of indexes for rows, columns and the values.

**Warning:** matrix = TRUE is **not** recommended, unless the order n be small. This matrix can require a huge amount of storage.

# Value

Returns an  $n^2$  by  $n^2$  matrix (if requested).

# References

Abadir, K.M., Magnus, J.R. (2005). Matrix Algebra. Cambridge University Press.

Magnus, J.R., Neudecker, H. (2007). *Matrix Differential Calculus with Applications in Statistics and Econometrics*, 3rd Edition. Wiley, New York.

# See Also

```
symm.info
```

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## **Examples**

```
z <- symmetrizer(n = 100)
object.size(z) # 319 Kb of storage

N100 <- symmetrizer(n = 100, matrix = TRUE) # time: < 2 secs
object.size(N100) # 800 Mb of storage, do not request this matrix!

# a small example
N3 <- symmetrizer(n = 3, matrix = TRUE)
a <- matrix(rep(c(2,4,6), each = 3), ncol = 3)
a
b <- 0.5 * (a + t(a))
b
v <- N3 %*% vec(a)
all(vec(b) == as.vector(v)) # vectors are equal!</pre>
```

vec

Vectorization of a matrix

# Description

This function returns a vector obtained by stacking the columns of x

# Usage

```
vec(x)
```

# Arguments

Х

a numeric matrix.

## Value

Let x be a n by m matrix, then vec(x) is a nm-dimensional vector.

# **Examples**

```
x <- matrix(rep(1:10, each = 10), ncol = 10)
x
y <- vec(x)
v</pre>
```

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vech

Vectorization the lower triangular part of a square matrix

# **Description**

This function returns a vector obtained by stacking the lower triangular part of a square matrix.

# Usage

```
vech(x)
```

# Arguments

Χ

a square matrix.

## Value

Let x be a n by n matrix, then vech(x) is a n(n+1)/2-dimensional vector.

# **Examples**

```
x <- matrix(rep(1:10, each = 10), ncol = 10)
x
y <- vech(x)
y</pre>
```

whitening

Whitening transformation

## **Description**

Applies the whitening transformation to a data matrix based on the Cholesky decomposition of the empirical covariance matrix.

# Usage

```
whitening(x, Scatter = NULL)
```

# **Arguments**

x vector or matrix of data with, say, p columns.

Scatter

covariance (or scatter) matrix  $(p \times p)$  of the distribution, must be positive definite. If NULL, the covariance matrix is estimated from the data.

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## Value

Returns the whitened data matrix  $Z = XW^T$ , where

$$\boldsymbol{W}^T \boldsymbol{W} = \boldsymbol{S}^{-1}.$$

with S the empirical covariance matrix.

#### References

Kessy, A., Lewin, A., Strimmer, K. (2018). Optimal whitening and decorrelation. *The American Statistician* **72**, 309-314.

# **Examples**

```
x <- iris[,1:4]
species <- iris[,5]
pairs(x, col = species) # plot of Iris
# whitened data
z <- whitening(x)
pairs(z, col = species) # plot of</pre>
```

wilson.hilferty

Wilson-Hilferty transformation

# **Description**

Returns the Wilson-Hilferty transformation of random variables with chi-squared distribution.

# Usage

```
wilson.hilferty(x)
```

#### **Arguments**

Х

vector or matrix of data with, say, p columns.

### **Details**

Let  $F=D^2/p$  be a random variable, where  $D^2$  denotes the squared Mahalanobis distance defined as

$$D^2 = (\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})$$

Thus the Wilson-Hilferty transformation is given by

$$z = \frac{F^{1/3} - (1 - \frac{2}{9p})}{(\frac{2}{9p})^{1/2}}$$

and z is approximately distributed as a standard normal distribution. This is useful, for instance, in the construction of QQ-plots.

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# References

Wilson, E.B., and Hilferty, M.M. (1931). The distribution of chi-square. *Proceedings of the National Academy of Sciences of the United States of America* **17**, 684-688.

# See Also

```
cov, Mahalanobis
```

# **Examples**

```
x <- iris[,1:4]
z <- wilson.hilferty(x)
par(pty = "s")
qqnorm(z, main = "Transformed distances Q-Q plot")
abline(c(0,1), col = "red", lwd = 2, lty = 2)</pre>
```

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