Package ‘subselect’

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Title Selecting Variable Subsets
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Description A collection of functions which (i) assess the quality of variable subsets as surro-
gates for a full data set, in either an exploratory data analysis or in the context of a multivari-
ate linear model, and (ii) search for subsets which are optimal under various criteria. Theoreti-
cal support for the heuristic search methods and exploratory data analysis crite-
ria is in Cadima, Cerdeira, Minhoto (2003, <doi:10.1016/j.csda.2003.11.001>). Theoretical sup-
port for the leap and bounds algorithm and the criteria for the general multivariate lin-
ear model is in Duarte Silva (2001, <doi:10.1006/jmva.2000.1920>). There is a package vi-
gnette "subselect", which includes additional references.
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Description

Given a set of variables, a Simulated Annealing algorithm seeks a k-variable subset which is optimal, as a surrogate for the whole set, with respect to a given criterion.

Usage

```r
anneal(mat, kmin, kmax = kmin, nsol = 1, niter = 1000, exclude = NULL, include = NULL, improvement = TRUE, setseed = FALSE, cooling = 0.05, temp = 1, coolfreq = 1, criterion = "default", pcindices = "first_k", initialsol=NULL, force=FALSE, H=NULL, r=0, tolval=1000*.Machine$double.eps,tolsym=1000*.Machine$double.eps)
```

Arguments

- `mat`: a covariance/correlation, information or sums of squares and products matrix of the variables from which the k-subset is to be selected. See the Details section below.
- `kmin`: the cardinality of the smallest subset that is wanted.
- `kmax`: the cardinality of the largest subset that is wanted.
- `nsol`: the number of initial/final subsets (runs of the algorithm).
- `niter`: the number of iterations of the algorithm for each initial subset.
- `exclude`: a vector of variables (referenced by their row/column numbers in matrix `mat`) that are to be forcibly excluded from the subsets.
- `include`: a vector of variables (referenced by their row/column numbers in matrix `mat`) that are to be forcibly included in the subsets.
improvement  a logical variable indicating whether or not the best final subset (for each cardinality) is to be passed as input to a local improvement algorithm (see function improve).

setseed  logical variable indicating whether to fix an initial seed for the random number generator, which will be re-used in future calls to this function whenever setseed is again set to TRUE.

cooling  variable in the $[0,1[$ interval indicating the rate of geometric cooling for the Simulated Annealing algorithm.

temp  positive variable indicating the initial temperature for the Simulated Annealing algorithm.

coolfreq  positive integer indicating the number of iterations of the algorithm between coolings of the temperature. By default, the temperature is cooled at every iteration.

criterion  Character variable, which indicates which criterion is to be used in judging the quality of the subsets. Currently, the "RM", "RV", "GCD", "Tau2", "Xi2", "Zeta2", "ccr12" and "Wald" criteria are supported (see the Details section, the References and the links rm.coef, rv.coef, gcd.coef, tau2.coef, xi2.coef, zeta2.coef and ccr12.coef for further details). The default criterion is "Rm" if parameter $r$ is zero (exploratory and PCA problems), "Wald" if $r$ is equal to one and mat has a "FisherI" attribute set to TRUE (generalized linear models), and "Tau2" otherwise (multivariate linear model framework).

pcindices  either a vector of ranks of Principal Components that are to be used for comparison with the k-variable subsets (for the GCD criterion only, see gcd.coef) or the default text first_k. The latter will associate PCs 1 to $k$ with each cardinality $k$ that has been requested by the user.

initialsol  vector, matrix or 3-d array of initial solutions for the simulated annealing search. If a single cardinality is required, initialsol may be a vector of length $k$, in which case it is used as the initial solution for all $n$sol final solutions that are requested; a $1 \times k$ matrix (as produced by the $bestsets$ output value of the algorithm functions anneal, genetic, or improve), or a $1 \times k \times 1$ array (as produced by the $subsets$ output value), in which case it will be treated as the above k-vector; or an $n$sol $x$ $k$ matrix, or $n$sol $x$ $k$ $x$ 3-d array, in which case each row (dimension 1) will be used as the initial solution for each of the $n$sol final solutions requested. If more than one cardinality is requested, initialsol can be a length$(kmin:kmax)$ x $kmax$ matrix (as produced by the $bestsets$ option of the algorithm functions), in which case each row will be replicated to produced the initial solution for all $n$sol final solutions requested in each cardinality, or a $n$sol $x$ $kmax$ x length$(kmin:kmax)$ 3-d array (as produced by the $subsets$ output option), in which case each row (dimension 1) is interpreted as a different initial solution.

If the exclude and/or include options are used, initialsol must also respect those requirements.

force  a logical variable indicating whether, for large data sets (currently $p > 400$) the algorithm should proceed anyways, regardless of possible memory problems which may crash the R session.
Effect description matrix. Not used with the RM, RV or GCD criteria, hence the NULL default value. See the Details section below.

**r**
Expected rank of the effects (H) matrix. Not used with the RM, RV or GCD criteria. See the Details section below.

**tolval**
The tolerance level for the reciprocal of the 2-norm condition number of the correlation/covariance matrix, i.e., for the ratio of the smallest to the largest eigenvalue of the input matrix. Matrices with a reciprocal of the condition number smaller than tolval will activate a restricted-search for well conditioned subsets.

**tolsym**
The tolerance level for symmetry of the covariance/correlation/total matrix and for the effects (H) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes \((A + t(A))/2\).

**Details**

An initial k-variable subset (for k ranging from kmin to kmax) of a full set of p variables is randomly selected and passed on to a Simulated Annealing algorithm. The algorithm then selects a random subset in the neighbourhood of the current subset (neighbourhood of a subset S being defined as the family of all k-variable subsets which differ from S by a single variable), and decides whether to replace the current subset according to the Simulated Annealing rule, i.e., either (i) always, if the alternative subset’s value of the criterion is higher; or (ii) with probability

\[
\exp \frac{ac - cc}{t}
\]

if the alternative subset’s value of the criterion (ac) is lower than that of the current solution (cc), where the parameter t (temperature) decreases throughout the iterations of the algorithm. For each cardinality k, the stopping criterion for the algorithm is the number of iterations (niter) which is controlled by the user. Also controlled by the user are the initial temperature (temp) the rate of geometric cooling of the temperature (cooling) and the frequency with which the temperature is cooled, as measured by coolfreq, the number of iterations after which the temperature is multiplied by 1-cooling.

Optionally, the best k-variable subset produced by Simulated Annealing may be passed as input to a restricted local search algorithm, for possible further improvement.

The user may force variables to be included and/or excluded from the k-subsets, and may specify initial solutions.

For each cardinality k, the total number of calls to the procedure which computes the criterion values is nsol x (niter + 1). These calls are the dominant computational effort in each iteration of the algorithm.

In order to improve computation times, the bulk of computations is carried out by a Fortran routine. Further details about the Simulated Annealing algorithm can be found in Reference 1 and in the comments to the Fortran code (in the src subdirectory for this package). For datasets with a very large number of variables (currently p > 400), it is necessary to set the force argument to TRUE for the function to run, but this may cause a session crash if there is not enough memory available.
The function checks for ill-conditioning of the input matrix (specifically, it checks whether the ratio of the input matrix’s smallest and largest eigenvalues is less than tolval). For an ill-conditioned input matrix, the search is restricted to its well-conditioned subsets. The function trim.matrix may be used to obtain a well-conditioned input matrix.

In a general descriptive (Principal Components Analysis) setting, the three criteria Rm, Rv and Gcd can be used to select good k-variable subsets. Arguments H and r are not used in this context. See references [1] and [2] and the Examples for a more detailed discussion.

In the setting of a multivariate linear model, \( X = A \Psi + U \), criteria Ccr12, Tau2, Xi2 and Zeta2 can be used to select subsets according to their contribution to an effect characterized by the violation of a reference hypothesis, \( C \Psi = 0 \) (see reference [3] for further details). In this setting, arguments mat and H should be set respectively to the usual Total (Hypothesis + Error) and Hypothesis, Sum of Squares and Cross-Products (SSCP) matrices. Argument r should be set to the expected rank of H. Currently, for reasons of computational efficiency, criterion Ccr12 is available only when \( r \leq 3 \). Particular cases in this setting include Linear Discriminant Analysis (LDA), Linear Regression Analysis (LRA), Canonical Correlation Analysis (CCA) with one set of variables fixed and several extensions of these and other classical multivariate methodologies.

In the setting of a generalized linear model, criterion Wald can be used to select subsets according to the (lack of) significance of the discarded variables, as measured by the respective Wald’s statistic (see reference [4] for further details). In this setting arguments mat and H should be set respectively to FI and FI %*% b %*% t(b) %*% FI, where b is a column vector of variable coefficient estimates and FI is an estimate of the corresponding Fisher information matrix.

The auxiliary functions lmHmat, ldaHmat glhHmat and glmHmat are provided to automatically create the matrices mat and H in all the cases considered.

**Value**

A list with five items:

- **subsets**
  
  An nsol x kmax x length(kmin:kmax) 3-dimensional array, giving for each cardinality (dimension 3) and each solution (dimension 1) the list of variables (referenced by their row/column numbers in matrix mat) in the subset (dimension 2). (For cardinalities smaller than kmax, the extra final positions are set to zero).

- **values**
  
  An nsol x length(kmin:kmax) matrix, giving for each cardinality (columns), the criterion values of the nsol (rows) subsets obtained.

- **bestvalues**
  
  A length(kmin:kmax) vector giving the best values of the criterion obtained for each cardinality. If improvement is TRUE, these values result from the final restricted local search algorithm (and may therefore exceed the largest value for that cardinality in values).

- **bestsets**
  
  A length(kmin:kmax) x kmax matrix, giving, for each cardinality (rows), the variables (referenced by their row/column numbers in matrix mat) in the best k-subset that was found.

- **call**

  The function call which generated the output.

**References**


See Also

`rm.coef`, `rv.coef`, `gcd.coef`, `tau2.coef`, `xi2.coef`, `zeta2.coef`, `ccr12.coef`, `genetic`, `anneal`, `eleaps`, `trim.matrix`, `lmHmat`, `ldaHmat`, `glhHmat`, `glmHmat`.

Examples

```r
## --------------------------------------------------------------------
## ## (1) For illustration of use, a small data set with very few iterations
## of the algorithm, using the RM criterion.
##
## data(swiss)
## anneal(cor(swiss),2,3,nsol=4,niter=10,criterion="RM")
##
##$subsets
## .. , Card.2
##   #
##   # Solution 1 3 6 0
##   Solution 2 4 5 0
##   Solution 3 1 2 0
##   Solution 4 3 6 0
##   #
##   #, , Card.3
##   #
##   # Solution 1 4 5 6
##   Solution 2 3 5 6
##   Solution 3 3 4 6
##   Solution 4 4 5 6
##   #
##
##$values
##   card.2 card.3
##   Solution 1 0.8016409 0.9043760
##   Solution 2 0.7982296 0.8769672
##   Solution 3 0.7945390 0.8777509
##   Solution 4 0.8016409 0.9043760
##
##$bestvalues
```
## Card.2 Card.3
##0.8016409 0.9043760
##
##$bestsets
## Var.1 Var.2 Var.3
##Card.2 3 6 0
##Card.3 4 5 6
##
##$call
##anneal(cor(swiss), 2, 3, nsol = 4, niter = 10, criterion = "RM")
##
## (2) An example excluding variable number 6 from the subsets.
##
## data(swiss)
anneal(cor(swiss),2,3,nsol=4,niter=10,criterion="RM",exclude=c(6))

##$subsets
## , , Card.2
##
## Var.1 Var.2 Var.3
##Solution 1 4 5 0
##Solution 2 4 5 0
##Solution 3 4 5 0
##Solution 4 4 5 0
##
## , , Card.3
##
## Var.1 Var.2 Var.3
##Solution 1 1 2 5
##Solution 2 1 2 5
##Solution 3 1 2 5
##Solution 4 1 5 0
##
##$values
## card.2 card.3
##Solution 1 0.7982296 0.8791856
##Solution 2 0.7982296 0.8791856
##Solution 3 0.7982296 0.8791856
##Solution 4 0.7982296 0.8686515

##$bestvalues
## Card.2 Card.3
##0.7982296 0.8791856

##$bestsets
## Var.1 Var.2 Var.3
##Card.2 4 5 0
##Card.3 1 2 5
## $call
## anneal(cor(swiss), 2, 3, nsol = 4, niter = 10, criterion = "RM",
## exclude=c(6))

## (3) An example specifying initial solutions: using the subsets produced
## by simulated annealing for one criterion (RM, by default) as initial
## solutions for the simulated annealing search with a different criterion.

data(swiss)
rmresults<-anneal(cor(swiss),2,3,nsol=4,niter=10, setseed=TRUE)
anneal(cor(swiss),2,3,nsol=4,niter=10,criterion="gcd",
initialsol=rmresults$subsets)

## $subsets
## , , Card.2
##    Var.1 Var.2 Var.3
##Solution 1  3  6  0
##Solution 2  3  6  0
##Solution 3  3  6  0
##Solution 4  3  6  0
##
## , , Card.3
##    Var.1 Var.2 Var.3
##Solution 1  4  5  6
##Solution 2  4  5  6
##Solution 3  3  4  6
##Solution 4  4  5  6
##
## $values
## card.2 card.3
##Solution 1  0.8487026  0.9253720
##Solution 2  0.8487026  0.9253720
##Solution 3  0.8487026  0.7988640
##Solution 4  0.8487026  0.9253720

## $bestvalues
## Card.2 Card.3
##0.8487026 0.9253720

## $bestsets
## Var.1 Var.2 Var.3
##Card.2 3 6 0
##Card.3 4 5 6

## $call
## anneal(cor(swiss), 2, 3, nsol = 4, niter = 10, criterion = "gcd",
## initialsol = rmresults$subsets)
(4) An example of subset selection in the context of Multiple Linear Regression. Variable 5 (average car price) in the Cars93 MASS library data set is regressed on 13 other variables. A best subset of linear predictors is sought, using the "TAU_2" criterion which, in the case of a Linear Regression, is merely the standard Coefficient of Determination, $R^2$ (like the other three criteria for the multivariate linear hypothesis, "XI_2", "CCR1_2" and "ZETA_2").

```r
library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,5])
names(Cars93[,5,drop=FALSE])
## [1] "Price"
colnames(CarsHmat$mat)
## [1] "MPG.city"   "MPG.highway"  "EngineSize"
## [4] "Horsepower"  "RPM"     "Rev.per.mile"
## [7] "Fuel.tank.capacity" "Passengers"  "Length"
## [10] "Wheelbase"    "Width"     "Turn.circle"
## [13] "Weight"

anneal(CarsHmat$mat, kmin=4, kmax=6, H=CarsHmat$H, r=1, crit="tau2")
```

```
# $subsets
# , , Card.4
#
# Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
# Solution 1  4  5  10  11  0  0
# #
# , , Card.5
# #
# Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
# Solution 1  4  5  10  11  12  0
# #
# , , Card.6
# #
# Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
# Solution 1  4  5  9  10  11  12
# #
# # $values
# # card.4 card.5 card.6
# # Solution 1 0.7143794 0.7241457 0.731015
# #
# # $bestvalues
# # Card.4 Card.5 Card.6
# # 0.7143794 0.7241457 0.731015
```
## $bestsets
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Card.4 4 5 10 11 0 0
## Card.5 4 5 10 11 12 0
## Card.6 4 5 9 10 11 12
##
## $call
## anneal(mat = CarsHmat$mat, kmin = 4, kmax = 6, criterion = "xi2",
## H = CarsHmat$H, r = 1)
##
## (5) A Linear Discriminant Analysis example with a very small data set.
## We consider the Iris data and three groups, defined by species (setosa,
## versicolor and virginica). The goal is to select the 2- and 3-variable
## subsets that are optimal for the linear discrimination (as measured
## by the "CCR1_2" criterion).

data(iris)
irisHmat <- ldaHmat(iris[1:4],iris$Species)
anneal(irisHmat$mat,kmin=2,kmax=3,H=irisHmat$H,r=2,crit="ccr12")

## $subsets
## , , Card.2
## #
## # Var.1 Var.2 Var.3
## # Solution 1 1 3 0
## #
## , , Card.3
## #
## # Var.1 Var.2 Var.3
## # Solution 1 2 3 4
## #
## # $values
## # card.2 card.3
## # Solution 1 0.9589055 0.967897
## #
## $bestvalues
## Card.2 Card.3
## 0.9589055 0.9678971
##
## $bestsets
## # Var.1 Var.2 Var.3
## # Card.2 1 3 0
## # Card.3 2 3 4
## #
## $call
## # anneal(irisHmat$mat,kmin=2,kmax=3,H=irisHmat$H,r=2,crit="ccr12")
## #
(6) An example of subset selection in the context of a Canonical Correlation Analysis. Two groups of variables within the Cars93 MASS library data set are compared. The goal is to select 4- to 6-variable subsets of the 13-variable 'X' group that are optimal in terms of preserving the canonical correlations, according to the "XI_2" criterion (Warning: the 3-variable 'Y' group is kept intact; subset selection is carried out in the 'X' group only). The 'tolsym' parameter is used to relax the symmetry requirements on the effect matrix H which, for numerical reasons, is slightly asymmetric. Since corresponding off-diagonal entries of matrix H are different, but by less than tolsym, H is replaced by its symmetric part: (H+t(H))/2.

library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,4:6])
names(Cars93[,4:6])
colnames(CarsHmat$mat)
## [1] "MPG.city" "MPG.highway" "EngineSize" 
## [4] "Horsepower" "RPM" "Rev.per.mile" 
## [7] "Fuel.tank.capacity" "Passengers" "Length" 
## [10] "Wheelbase" "Width" "Turn.circle" 
## [13] "Weight"

anneal(CarsHmat$mat, kmin=4, kmax=6, H=CarsHmat$H, r=CarsHmat$r, crit="tau2", tolsym=1e-9)

## $subsets
## , , Card.4
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 4 9 10 11 0 0
## , , Card.5
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 3 4 9 10 11 0
## , , Card.6
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 3 4 5 9 10 11
## $values
## card.4 card.5 card.6
## Solution 1 0.2818772 0.2943742 0.3057831
## $bestvalues
## Card.4   Card.5   Card.6  
## 0.2818772 0.2943742 0.3057831
## 
## $bestsets
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6  
## Card.4   4   9   10  11   0   0  
## Card.5   3   4   9   10  11   0  
## Card.6   3   4   5   9  10  11  
## 
## $call
## anneal(mat = CarsHmat$mat, kmin = 4, kmax = 6, criterion = "xi2",  
## H = CarsHmat$H, r = CarsHmat$r, tolsym = 1e-09)
## 
## Warning message:
## The effect description matrix (H) supplied was slightly asymmetric:  
## symmetric entries differed by up to 3.63797880709171e-12.  
## (less than the 'tolsym' parameter).  
## The H matrix has been replaced by its symmetric part.  
## in: validnovcrit(mat, criterion, H, r, p, tolval, tolsym)
## 
## (7) An example of variable selection in the context of a logistic  
## regression model. We consider the last 100 observations of  
## the iris data set (versicolor and virginica species) and try  
## to find the best variable subsets for the model that takes species  
## as response variable.
##
data(iris)
iris2sp <- iris[iris$Species != "setosa",]
logrfit <- glm(Species ~ Sepal.Length + Sepal.Width + Petal.Length + Petal.Width,  
iris2sp, family=binomial)
Hmat <- glmHmat(logrfit)
anneal(Hmat$mat,1,3,H=Hmat$H,r=1,criterion="Wald")

## $subsets
## , , Card.1  
##       Var.1 Var.2 Var.3  
## Solution 1 4   0   0  
## , , Card.2  
##       Var.1 Var.2 Var.3  
## Solution 1 1   3   0  
## , , Card.3  
##       Var.1 Var.2 Var.3  
## Solution 1 2   3   4
## $values
## card.1  card.2  card.3
## Solution 1  4.894554  3.522885  1.060121

## $bestvalues
## Card.1  Card.2  Card.3
## 4.894554  3.522885  1.060121

## $bestsets
## Var.1  Var.2  Var.3
## Card.1  4    0    0
## Card.2  1    3    0
## Card.3  2    3    4

## $call
## anneal(mat = Hmat$mat, kmin = 1, kmax = 3, criterion = "Wald",
##         H = Hmat$H, r = 1)

# It should be stressed that, unlike other criteria in the
# subselect package, the Wald criterion is not bounded above by
# 1 and is a decreasing function of subset quality, so that the
# 3-variable subsets do, in fact, perform better than their smaller-sized
# counterparts.

---

**ccr12.coef**  

*First Squared Canonical Correlation for a multivariate linear hypothesis*

---

**Description**

Computes the first squared canonical correlation. The maximization of this criterion is equivalent to the maximization of the Roy first root.

**Usage**

```r
ccr12.coef(mat, H, r, indices,
           tolval=10*.Machine$double.eps, tolsym=1000*.Machine$double.eps)
```

**Arguments**

- `mat`  
  the Variance or Total sums of squares and products matrix for the full data set.

- `H`  
  the Effect description sums of squares and products matrix (defined in the same way as the `mat` matrix).

- `r`  
  the Expected rank of the `H` matrix. See the Details section below.
indices a numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different $k$-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.

tolval the tolerance level to be used in checks for ill-conditioning and positive-definiteness of the 'total' and 'effects' (H) matrices. Values smaller than tolval are considered equivalent to zero.

tolsym the tolerance level for symmetry of the covariance/correlation/total matrix and for the effects (H) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes $(A+t(A))/2$.

Details

Different kinds of statistical methodologies are considered within the framework, of a multivariate linear model:

$$X = A\Psi + U$$

where $X$ is the (nxp) data matrix of original variables, $A$ is a known (nxp) design matrix, $\Psi$ an (qxp) matrix of unknown parameters and $U$ an (nxp) matrix of residual vectors. The $ccr_1^2$ index is related to the traditional test statistic (the Roy first root) and measures the contribution of each subset to an Effect characterized by the violation of a linear hypothesis of the form $C\Psi = 0$, where $C$ is a known coefficient matrix of rank $r$. The Roy first root is the first eigen value of $HE^{-1}$, where $H$ is the Effect matrix and $E$ is the Error matrix. The index $ccr_1^2$ is related to the Roy first root ($\lambda_1$) by:

$$ccr_1^2 = \frac{\lambda_1}{1 + \lambda_1}$$

The fact that indices can be a matrix or 3-d array allows for the computation of the $ccr_1^2$ values of subsets produced by the search functions `anneal`, `genetic`, `improve` and `anneal` (whose output option `$subsets` are matrices or 3-d arrays), using a different criterion (see the example below).

Value

The value of the $ccr_1^2$ coefficient.

Examples

```r
## 1) A Linear Discriminant Analysis example with a very small data set.
## We considered the Iris data and three groups,
## defined by species (setosa, versicolor and virginica).

data(iris)
irisHmat <- ldaHmat(iris[1:4], iris$Species)
ccr12.coef(irisHmat$mat, H=irisHmat$H, r=2, c(1,3))
## [1] 0.9589055
```
eleaps

---

## Example computing the value of the ccr1_2 criteria for two subsets produced when the anneal function attempted to optimize the zeta_2 criterion (using an absurdly small number of iterations).

```r
zetaresults <- anneal(irisHmat$mat, 2, nsol = 2, niter = 2, criterion = "zeta2", H = irisHmat$H, r = 2)
ccr12.coef(irisHmat$mat, H = irisHmat$H, r = 2, zetaresults$subsets)
```

Card.2
Solution 1 0.9526304
Solution 2 0.9558787
---

### Description

An exact Algorithm for optimizing criteria that measure the quality of k-dimensional variable subsets as approximations to a given set of variables, or to a set of its Principal Components.

### Usage

```r
eleaps(mat, kmin = length(include) + 1, kmax = ncol(mat) - length(exclude) - 1, nsol = 1, exclude = NULL, include = NULL, criterion = "default", pcindices = "first_k", timelimit = 15, H = NULL, r = 0, tolval = 1000 * .Machine$double.eps, tolsym = 1000 * .Machine$double.eps, maxaperr = 1E-4)
```

### Arguments

- **mat**: A covariance/correlation, information or sums of squares and products matrix of the variables from which the k-subset is to be selected. See the Details section below.
- **kmin**: The cardinality of the smallest subset that is wanted.
- **kmax**: The cardinality of the largest subset that is wanted.
- **nsol**: The number of different subsets of each cardinality that are requested.
- **exclude**: A vector of variables (referenced by their row/column numbers in matrix mat) that are to be forcibly excluded from the subsets.
- **include**: A vector of variables (referenced by their row/column numbers in matrix mat) that are to be forcibly included in the subsets.
criterion  Character variable, which indicates which criterion is to be used in judging the quality of the subsets. Currently, the "Rm", "Rv", "Gcd", "Tau2", "Xi2", "Zeta2", "Ccr12" and "Wald" criteria are supported (see the Details section, the References and the links rm.coef, rv.coef, gcd.coef, tau2.coef, xi2.coef, zeta2.coef, ccr12.coef and wald.coef for further details). The default criterion is "Rm" if parameter r is zero (exploratory and PCA problems), "Wald" if r is equal to one and mat has a "FisherI" attribute set to TRUE (generalized linear models), and "Tau2" otherwise (multivariate linear model framework).

pcindices  either a vector of ranks of Principal Components that are to be used for comparison with the k-variable subsets (for the Gcd criterion only, see gcd.coef) or the default text first_k. The latter will associate PCs 1 to k that has been requested by the user.

timelimit  a user specified limit (in seconds) for the maximum time allowed to conduct the search. After this limit is exceeded, eleaps exits with a warning message stating that it was not possible to find the optimal subsets within the allocated time.

H  Effect description matrix. Not used with the Rm, Rv or Gcd criteria, hence the NULL default value. See the Details section below.

r  Expected rank of the effects (H) matrix. Not used with the Rm, Rv or Gcd criteria. See the Details section below.

tolval  the tolerance level for the reciprocal of the 2-norm condition number of the correlation/covariance or sums of squares matrix, i.e., for the ratio of the smallest to the largest eigenvalue of the input matrix. Matrices with a reciprocal of the condition number smaller than tolval will activate a restricted-search (for well conditioned sets as defined by the value of the maxaperr argument) algorithm.

tolsym  the tolerance level for symmetry of the covariance/correlation/total matrix and for the effects (H) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes (A+t(A))/2.

maxaperr  the tolerance level for the relative rounding error of the criterion. When a restricted search in employed subsets where a first order estimate of this error is higher than maxaperr will be excluded from the analysis.

Details

For each cardinality k (with k ranging from kmin to kmax), eleaps performs a branch and bound search for the best n.sol variable subsets according to a specified criterion. Leaps implements Duarte Silva's adaptation (references [2] and [3]) of Furnival and Wilson's Leaps and Bounds Algorithm (reference [4]) for variable selection in Regression Analysis. If the search is not completed within a user defined time limit, eleaps exits with a warning message.

The user may force variables to be included and/or excluded from the k-subsets.

In order to improve computation times, the bulk of computations are carried out by C++ routines. Further details about the Algorithm can be found in references [2] and [3] and in the comments to the C++ code. A discussion of the criteria considered can be found in References [1] and [3].
The function checks for ill-conditioning of the input matrix (specifically, it checks whether the ratio of the input matrix’s smallest and largest eigenvalues is less than tolval). For an ill-conditioned input matrix, the search is restricted to its well-conditioned subsets. The function `trim.matrix` may be used to obtain a well-conditioned input matrix.

In a general descriptive (Principal Components Analysis) setting, the three criteria Rm, Rv and Gcd can be used to select good k-variable subsets. Arguments H and r are not used in this context. See reference [1] and the Examples for a more detailed discussion.

In the setting of a multivariate linear model, \( X = A\Psi + U \), criteria Ccr12, Tau2, Xi2 and Zeta2 can be used to select subsets according to their contribution to an effect characterized by the violation of a reference hypothesis, \( C\Psi = 0 \) (see reference [3] for further details). In this setting, arguments mat and H should be set respectively to the usual Total (Hypothesis + Error) and Hypothesis, Sum of Squares and Cross-Products (SSCP) matrices. Argument r should be set to the expected rank of H. Currently, for reasons of computational efficiency, criterion Ccr12 is available only when \( r \leq 3 \). Particular cases in this setting include Linear Discriminant Analysis (LDA), Linear Regression Analysis (LRA), Canonical Correlation Analysis (CCA) with one set of variables fixed, and several extensions of these and other classical multivariate methodologies.

In the setting of a generalized linear model, criterion Wald can be used to select subsets according to the (lack of) significance of the discarded variables, as measured by the respective Wald’s statistic (see reference [5] for further details). In this setting arguments mat and H should be set respectively to FI and \( FI \%\% b \%\% t(b) \%\% FI \), where \( b \) is a column vector of variable coefficient estimates and \( FI \) is an estimate of the corresponding Fisher information matrix.

The auxiliary functions `lmHmat`, `ldaHmat`, `glmHmat` and `glmHmat` are provided to automatically create the matrices mat and H in all the cases considered.

**Value**

A list with five items:

- **subsets** An \( nsol \times kmax \times \text{length}(kmin:kmax) \) 3-dimensional array, giving for each cardinality (dimension 3) and each solution (dimension 1) the list of variables (referenced by their row/column numbers in matrix mat) in the subset (dimension 2). (For cardinalities smaller than \( kmax \), the extra final positions are set to zero).

- **values** An \( nsol \times \text{length}(kmin:kmax) \) matrix, giving for each cardinality (columns), the criterion values of the best \( nsol \) (rows) subsets according to the chosen criterion.

- **bestvalues** A \( \text{length}(kmin:kmax) \) vector giving the overall best values of the criterion for each cardinality.

- **bestsets** A \( \text{length}(kmin:kmax) \times kmax \) matrix, giving, for each cardinality (rows), the variables (referenced by their row/column numbers in matrix mat) in the best k-subset.

- **call** The function call which generated the output.

**References**


See Also

`rm.coef`, `rv.coef`, `gcd.coef`, `tau2.coef`, `wald.coef`, `z2.coef`, `cc12.coef`, `anneal`, `genetic`, `anneal`, `trim.matrix`, `lmHmat`, `ldaHmat`, `glmHmat`, `glmHmat`.

Examples

```r
## --------------------------------------------------------------------
##
## 1) For illustration of use, a small data set.
## Subsets of variables of all cardinalities are sought using the
## RM criterion.
##
## data(swiss)
eleaps(cor(swiss),nsol=3, criterion="RM")

## Subsets
## , , Card.1
##
## Var.1 Var.2 Var.3 Var.4 Var.5
##Solution 1 3 0 0 0 0
##Solution 2 1 0 0 0 0
##Solution 3 4 0 0 0 0
##
## , , Card.2
##
## Var.1 Var.2 Var.3 Var.4 Var.5
##Solution 1 3 6 0 0 0
##Solution 2 4 5 0 0 0
##Solution 3 1 2 0 0 0
##
## , , Card.3
##
## Var.1 Var.2 Var.3 Var.4 Var.5
##Solution 1 4 5 6 0 0
##Solution 2 1 2 5 0 0
##Solution 3 3 4 6 0 0
##
## , , Card.4
##
## Var.1 Var.2 Var.3 Var.4 Var.5
```
eleaps

```
##Solution 1  2  4  5  6  0
##Solution 2  1  2  5  6  0
##Solution 3  1  4  5  6  0
##
##, , Card.5
##
##  Var.1  Var.2  Var.3  Var.4  Var.5
##Solution 1  1  2  3  5  6
##Solution 2  1  2  4  5  6
##Solution 3  2  3  4  5  6
##
##$values
## card.1  card.2  card.3  card.4  card.5
##Solution 1  0.6729689  0.8016409  0.9043760  0.9510757  0.9804629
##Solution 2  0.6286185  0.7982296  0.8791856  0.9506434  0.9776338
##Solution 3  0.6286130  0.7945390  0.8777509  0.9395708  0.9752551
##
##$bestvalues
## Card.1  Card.2  Card.3  Card.4  Card.5
##0.6729689  0.8016409  0.9043760  0.9510757  0.9804629
##
##$bestsets
## Var.1  Var.2  Var.3  Var.4  Var.5
##Card.1  3 0 0 0 0
##Card.2  3 6 0 0 0
##Card.3  4 5 6 0 0
##Card.4  2 4 5 6 0
##Card.5  1 2 3 5 6
##
##$call
##eleaps(cor(swiss), nsol = 3, criterion="RM")
```

---

```
## 2) Asking only for 2- and 3-dimensional subsets and excluding
## variable number 6.
##
data(swiss)
eleaps(cor(swiss),2,3,exclude=6,nsol=3,criterion="rm")
```

```
##$subsets
##, , Card.2
##
##  Var.1  Var.2  Var.3
##Solution 1  4  5  0
##Solution 2  1  2  0
##Solution 3  1  3  0
##
##, , Card.3
```
```
## Solution 1 1 2 5
## Solution 2 1 4 5
## Solution 3 2 4 5
##
## $values
card.2 card.3
Solution 1 0.7982296 0.8791856
Solution 2 0.7945390 0.8686515
Solution 3 0.7755232 0.8628693

## $bestvalues
Card.2 Card.3
0.7982296 0.8791856

## $bestsets
Card.2 4 5 0
Card.3 1 2 5

## $call
eleaps(cor(swiss), 2, 3, exclude = 6, nsol = 3, criterion = "gcd")
```

```
## 3) Searching for 2- and 3- dimensional subsets that best approximate
## the spaces generated by the first three Principal Components
##
## data(swiss)
eleaps(cor(swiss), 2, 3, exclude = 6, nsol = 3, criterion = "gcd", pcindices = 1:3)
```

```
## $subsets
,, Card.2
##
## Solution 1 4 5 0
## Solution 2 5 6 0
## Solution 3 4 6 0

,, Card.3
##
## Solution 1 4 5 0
## Solution 2 3 5 6
## Solution 3 2 5 6

## $values
```
## Solution 1 0.7831827 0.9253684
## Solution 2 0.7475630 0.8459302
## Solution 3 0.7383665 0.8243032

## bestvalues
## Card.2 Card.3
## 0.7831827 0.9253684

## bestsets
## Var.1 Var.2 Var.3
## Card.2 4 5 0
## Card.3 4 5 6

## call
eleaps(cor(swiss), 2, 3, criterion = "gcd", pcindices = 1:3, nsol = 3)

## 4) An example of subset selection in the context of Multiple Linear Regression. Variable 5 (average car price) in the Cars93 MASS library data set is regressed on 13 other variables. A best subset of linear predictors is sought, using the default criterion ("TAU_2") which, in the case of a Linear Regression, is merely the standard Coefficient of Determination, $R^2$ (as are the other three criteria for the multivariate linear hypothesis, "XI_2", "CCR1_2" and "ZETA_2").

library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,5])
names(Cars93[,5,drop=FALSE])
## [1] "Price"
colnames(CarsHmat$mat)
## [1] "MPG.city" "MPG.highway" "EngineSize"
## [4] "Horsepower" "RPM" "Rev.per.mile"
## [7] "Fuel.tank.capacity" "Passengers" "Length"
## [10] "Wheelbase" "Width" "Turn.circle"
## [13] "Weight"
eleaps(CarsHmat$mat, kmin=4, kmax=6, H=CarsHmat$H, r=1)

## $subsets
## , , Card.4
## ## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 4 5 10 11 0 0
## A Linear Discriminant Analysis example with a very small data set.
## We consider the Iris data and three groups, defined by species (setosa, versicolor and virginica). The goal is to select the 2- and 3-variable subsets that are optimal for the linear discrimination (as measured by the "CCR1_2" criterion).

data(iris)
irisHmat <- ldaHmat(iris[1:4],iris$Species)
eleaps(irisHmat$mat,kmin=2,kmax=3,H=irisHmat$H,r=2,crit="ccr12")

## $subsets
## , , Card.2
## Var.1 Var.2 Var.3
## Solution 1 1 3 0
## , , Card.3
## Var.1 Var.2 Var.3
## Solution 1 2 3 4

## $values
card.2 card.3
eleaps

## Solution 1 0.9589055 0.967897
## $bestvalues
## Card.2  Card.3
## 0.9589055 0.9678971
## $bestsets
## Var.1 Var.2 Var.3
## Card.2 1 3 0
## Card.3 2 3 4

## 6) An example of subset selection in the context of a Canonical Correlation Analysis. Two groups of variables within the Cars93 MASS library data set are compared. The goal is to select 4- to 6-variable subsets of the 13-variable 'X' group that are optimal in terms of preserving the canonical correlations, according to the "ZETA_2" criterion (Warning: the 3-variable 'Y' group is kept intact; subset selection is carried out in the 'X' group only). The 'tolsym' parameter is used to relax the symmetry requirements on the effect matrix $H$ which, for numerical reasons, is slightly asymmetric. Since corresponding off-diagonal entries of matrix $H$ are different, but by less than tolsym, $H$ is replaced by its symmetric part: $(H+t(H))/2$.

library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,4:6])

names(Cars93[,4:6])
colnames(CarsHmat$mat)
## [1] "MPG.city" "MPG.highway" "EngineSize"
## [4] "Horsepower" "RPM" "Rev.per.mile"
## [7] "Fuel.tank.capacity" "Passengers" "Length"
## [10] "Wheelbase" "Width" "Turn.circle"
## [13] "Weight"

eleaps(CarsHmat$mat, kmin=4, kmax=6, H=CarsHmat$H, r=3, crit="zeta2", tolsym=1e-9)

## $subsets
## , , Card.4
## #
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 3 4 10 11 0 0
##
7) An example of variable selection in the context of a logistic regression model. We consider the last 100 observations of the iris data set (versicolor an verginica species) and try to find the best variable subsets for the model that takes species as response variable.

data(iris)
iris2sp <- iris[iris$Species != "setosa",]
logrfit <- glm(Species ~ Sepal.Length + Sepal.Width + Petal.Length + Petal.Width, iris2sp,family=binomial)
Hmat <- glmHmat(logrfit)
eleaps(Hmat$mat,H=Hmat$H,r=1,criterion="Wald",nsol=3)

## $subsets
## , , Card.1
## Var.1 Var.2 Var.3
## Solution 1 4 0 0
## Solution 2 1 0 0
## Solution 3 3 0 0

## , , Card.2

## Var.1 Var.2 Var.3
## Solution 1 1 3 0
## Solution 2 3 4 0
## Solution 3 2 4 0

## , , Card.3

## Var.1 Var.2 Var.3
## Solution 1 2 3 4
## Solution 2 1 3 4
## Solution 3 1 2 3

## $values
## card.1 card.2 card.3
## Solution 1 4.894554 3.522885 1.060121
## Solution 2 5.147360 3.952538 2.224335
## Solution 3 5.161553 3.972410 3.522879

## $bestvalues
## Card.1 Card.2 Card.3
## 4.894554 3.522885 1.060121

## $bestsets
## Var.1 Var.2 Var.3
## Card.1 4 0 0
## Card.2 1 3 0
## Card.3 2 3 4

## $call
## eleaps(mat = Hmat$mat, nsol = 3, criterion = "Wald", H = Hmat$H,
## r = 1)
## *****************************************************************

# It should be stressed that, unlike other criteria in the
# subselect package, the Wald criterion is not bounded above by
# 1 and is a decreasing function of subset quality, so that the
# 3-variable subsets do, in fact, perform better than their smaller-sized
# counterparts.

---

**Sixty-two economic indicators from 99 Portuguese farms.**
Description

This data set is a very small subset of economic data regarding Portuguese farms in the mid-1990s, from Portugal’s Ministry of Agriculture.

Usage

\textit{farm}

Format

A 99x62 matrix. The 62 columns are numeric economic indicators, referenced by their database code. Monetary units are in thousands of Escudos (Portugal’s pre-Euro currency).

<table>
<thead>
<tr>
<th>Column Number</th>
<th>Column Name</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>[.1]</td>
<td>R15</td>
<td>1000 Escudos</td>
<td>Total Standard Gross Margins (SGM)</td>
</tr>
<tr>
<td>[.2]</td>
<td>R24</td>
<td>Hectares</td>
<td>Total land surface</td>
</tr>
<tr>
<td>[.3]</td>
<td>R35</td>
<td>Hectares</td>
<td>Total cultivated surface</td>
</tr>
<tr>
<td>[.4]</td>
<td>R36</td>
<td>Man Work Units</td>
<td>Total Man Work Units</td>
</tr>
<tr>
<td>[.5]</td>
<td>R46</td>
<td>1000 Escudos</td>
<td>Land Capital</td>
</tr>
<tr>
<td>[.6]</td>
<td>R59</td>
<td>1000 Escudos</td>
<td>Total Capital (without forests)</td>
</tr>
<tr>
<td>[.7]</td>
<td>R65</td>
<td>1000 Escudos</td>
<td>Total Loans and Debts</td>
</tr>
<tr>
<td>[.8]</td>
<td>R72</td>
<td>1000 Escudos</td>
<td>Total Investment</td>
</tr>
<tr>
<td>[.9]</td>
<td>R79</td>
<td>1000 Escudos</td>
<td>Subsidies for Investment</td>
</tr>
<tr>
<td>[10]</td>
<td>R86</td>
<td>1000 Escudos</td>
<td>Gross Plant Product Formation</td>
</tr>
<tr>
<td>[12]</td>
<td>R104</td>
<td>1000 Escudos</td>
<td>Current Subsidies</td>
</tr>
<tr>
<td>[13]</td>
<td>R110</td>
<td>1000 Escudos</td>
<td>Wheat Production</td>
</tr>
<tr>
<td>[14]</td>
<td>R111</td>
<td>1000 Escudos</td>
<td>Maize Production</td>
</tr>
<tr>
<td>[15]</td>
<td>R113</td>
<td>1000 Escudos</td>
<td>Other Cereals (except rice) Production</td>
</tr>
<tr>
<td>[16]</td>
<td>R114</td>
<td>1000 Escudos</td>
<td>Dried Legumes Production</td>
</tr>
<tr>
<td>[17]</td>
<td>R115</td>
<td>1000 Escudos</td>
<td>Potato Production</td>
</tr>
<tr>
<td>[18]</td>
<td>R116</td>
<td>1000 Escudos</td>
<td>Industrial horticulture and Melon Production</td>
</tr>
<tr>
<td>[19]</td>
<td>R117</td>
<td>1000 Escudos</td>
<td>Open-air horticultural Production</td>
</tr>
<tr>
<td>[20]</td>
<td>R118</td>
<td>1000 Escudos</td>
<td>Horticultural forcing Production</td>
</tr>
<tr>
<td>[21]</td>
<td>R119</td>
<td>1000 Escudos</td>
<td>Flower Production</td>
</tr>
<tr>
<td>[22]</td>
<td>R121</td>
<td>1000 Escudos</td>
<td>Sub-products Production</td>
</tr>
<tr>
<td>[23]</td>
<td>R122</td>
<td>1000 Escudos</td>
<td>Fruit Production</td>
</tr>
<tr>
<td>[24]</td>
<td>R123</td>
<td>1000 Escudos</td>
<td>Olive Production</td>
</tr>
<tr>
<td>[25]</td>
<td>R124</td>
<td>1000 Escudos</td>
<td>Wine Production</td>
</tr>
<tr>
<td>[26]</td>
<td>R125</td>
<td>1000 Escudos</td>
<td>Horses</td>
</tr>
<tr>
<td>[27]</td>
<td>R126</td>
<td>1000 Escudos</td>
<td>Bovines (excluding milk)</td>
</tr>
<tr>
<td>[28]</td>
<td>R127</td>
<td>1000 Escudos</td>
<td>Milk and dairy products</td>
</tr>
<tr>
<td>[29]</td>
<td>R129</td>
<td>1000 Escudos</td>
<td>Sheep</td>
</tr>
<tr>
<td>[30]</td>
<td>R132</td>
<td>1000 Escudos</td>
<td>Goats</td>
</tr>
<tr>
<td>[31]</td>
<td>R135</td>
<td>1000 Escudos</td>
<td>Pigs</td>
</tr>
<tr>
<td>[32]</td>
<td>R137</td>
<td>1000 Escudos</td>
<td>Birds</td>
</tr>
<tr>
<td>[33]</td>
<td>R140</td>
<td>1000 Escudos</td>
<td>Bees</td>
</tr>
<tr>
<td>[34]</td>
<td>R142</td>
<td>1000 Escudos</td>
<td>Other animals (except rabbits)</td>
</tr>
<tr>
<td>[35]</td>
<td>R144</td>
<td>1000 Escudos</td>
<td>Wood production</td>
</tr>
</tbody>
</table>
Source

Obtained directly from the source.

### gcd.coef

Computes Yanai’s GCD in the context of the variable-subset selection problem

**Description**

Computes Yanai’s Generalized Coefficient of Determination for the similarity of the subspaces spanned by a subset of variables and a subset of the full data set’s Principal Components.

**Usage**

```r
gcd.coef(mat, indices, pcindices = NULL)
```
Arguments
mat the full data set’s covariance (or correlation) matrix.
indices a numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different $k$-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.
pcindices a numerical vector of indices of Principal Components. By default, the first $k$ PCs are chosen, where $k$ is the cardinality of the subset of variables whose criterion value is being computed. If a vector of PCs is specified by the user, those PCs will be used for all cardinalities that were requested.

Details
Computes Yanai’s Generalized Coefficient of Determination for the similarity of the subspaces spanned by a subset of variables (specified by indices) and a subset of the full-data set’s Principal Components (specified by pcindices). Input data is expected in the form of a (co)variance or correlation matrix. If a non-square matrix is given, it is assumed to be a data matrix, and its correlation matrix is used as input. The number of variables ($k$) and of PCs ($q$) does not have to be the same.

Yanai’s GCD is defined as:

$$GCD = \frac{\text{tr}(P_v \cdot P_c)}{\sqrt{k \cdot q}}$$

where $P_v$ and $P_c$ are the matrices of orthogonal projections on the subspaces spanned by the $k$-variable subset and by the $q$-Principal Component subset, respectively.

This definition is equivalent to:

$$GCD = \frac{1}{\sqrt{kq}} \sum_i (r_m)_i^2$$

where $(r_m)_i$ stands for the multiple correlation between the $i$-th Principal Component and the $k$-variable subset, and the sum is carried out over the $q$ PCs ($i=1,...,q$) selected.

These definitions are also equivalent to the expression used in the code, which only requires the covariance (or correlation) matrix of the data under consideration.

The fact that indices can be a matrix or 3-d array allows for the computation of the GCD values of subsets produced by the search functions anneal, genetic and improve (whose output option $subsets$ are matrices or 3-d arrays), using a different criterion (see the example below).

Value
The value of the GCD coefficient.

References

Examples

```r
## An example with a very small data set.

data(iris3)
x <- iris3[, , 1]
gcd.coef(cor(x), c(1, 3))
## [1] 0.7666286
gcd.coef(cor(x), c(1, 3), pcindices = c(1, 3))
## [1] 0.584452
gcd.coef(cor(x), c(1, 3), pcindices = 1)
## [1] 0.6035127

## An example computing the GCDs of three subsets produced when the
## anneal function attempted to optimize the RV criterion (using an
## absurdly small number of iterations).

data(swiss)
rvresults <- anneal(cor(swiss), 2, nsol = 4, niter = 5, criterion = "Rv")
gcd.coef(cor(swiss), rvresults$subsets)
## Card. 2
## Solution 1  0.4962297
## Solution 2  0.7092591
## Solution 3  0.4748525
## Solution 4  0.4649259
```

---

**genetic**

*Genetic Algorithm searching for an optimal k-variable subset*

Description

Given a set of variables, a Genetic Algorithm algorithm seeks a k-variable subset which is optimal, as a surrogate for the whole set, with respect to a given criterion.

Usage

```r
genetic( mat, kmin, kmax = kmin, popsize = max(100, 2 * ncol(mat)), nger = 100, 
mutate = FALSE, mutprob = 0.01, maxclone = 5, exclude = NULL, 
include = NULL, improvement = TRUE, setseed = FALSE, criterion = "default", 
pcindices = "first_k", initialpop = NULL, force = FALSE, H = NULL, r = 0, 
tolval = 1000 *.Machine$double.eps, tolsym = 1000 *.Machine$double.eps)
```

Arguments

- **mat**
  a covariance/correlation, information or sums of squares and products matrix of the variables from which the k-subset is to be selected. See the Details section below.
kmin: the cardinality of the smallest subset that is wanted.
kmax: the cardinality of the largest subset that is wanted.
popsiz: integer variable indicating the size of the population.
nger: integer variable giving the number of generations for which the genetic algorithm will run.
mutate: logical variable indicating whether each child undergoes a mutation, with probability mutprob. By default, FALSE.
mutprob: variable giving the probability of each child undergoing a mutation, if mutate is TRUE. By default, 0.01. High values slow down the algorithm considerably and tend to replicate the same solution.
maxclone: integer variable specifying the maximum number of identical replicates (clones) of individuals that is acceptable in the population. Serves to ensure that the population has sufficient genetic diversity, which is necessary to enable the algorithm to complete the specified number of generations. However, even maxclone=0 does not guarantee that there are no repetitions: only the offspring of couples are tested for clones. If any such clones are rejected, they are replaced by a k-variable subset chosen at random, without any further clone tests.
exclude: a vector of variables (referenced by their row/column numbers in matrix mat) that are to be forcibly excluded from the subsets.
include: a vector of variables (referenced by their row/column numbers in matrix mat) that are to be forcibly included in the subsets.
improvement: a logical variable indicating whether or not the best final subset (for each cardinality) is to be passed as input to a local improvement algorithm (see function improve).
setseed: logical variable indicating whether to fix an initial seed for the random number generator, which will be re-used in future calls to this function whenever setseed is again set to TRUE.
criterion: Character variable, which indicates which criterion is to be used in judging the quality of the subsets. Currently, the "Rm", "Rv", "Gcd", "Tau2", "Xi2", "Zeta2", "ccr12" and "Wald" criteria are supported (see the Details section, the References and the links rm.coef, rv.coef, gcd.coef, tau2.coef, xi2.coef, zeta2.coef and ccr12.coef for further details). The default criterion is "Rm" if parameter r is zero (exploratory and PCA problems), "Wald" if r is equal to one and mat has a "FisherI" attribute set to TRUE (generalized linear models), and "Tau2" otherwise (multivariate linear model framework).
pcindices: either a vector of ranks of Principal Components that are to be used for comparison with the k-variable subsets (for the Gcd criterion only, see gcd.coef) or the default text first_k. The latter will associate PCs 1 to k with each cardinality k that has been requested by the user.
initialpop: vector, matrix or 3-d array of initial population for the genetic algorithm. If a single cardinality is required, initialpop may be a popsiz x k matrix or a popsiz x k x 1 array (as produced by the $subsets output value of any of the algorithm functions anneal, genetic, or improve). If more than one cardinality is requested, initialpop must be a popsiz x kmax x length(kmin:kmax) 3-d array (as produced by the $subsets output value).
If the exclude and/or include options are used, initialpop must also respect those requirements.

**force**

A logical variable indicating whether, for large data sets (currently $p > 400$) the algorithm should proceed anyways, regardless of possible memory problems which may crash the R session.

**$H$**

Effect description matrix. Not used with the Rm, Rv or Gcd criteria, hence the NULL default value. See the Details section below.

**$r$**

Expected rank of the effects ($H$) matrix. Not used with the Rm, Rv or Gcd criteria. See the Details section below.

**tolval**

The tolerance level for the reciprocal of the 2-norm condition number of the correlation/covariance matrix, i.e., for the ratio of the smallest to the largest eigenvalue of the input matrix. Matrices with a reciprocal of the condition number smaller than tolval will activate a restricted-search for well conditioned subsets.

**tolsym**

The tolerance level for symmetry of the covariance/correlation/total matrix and for the effects ($H$) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix $A$ becomes $(A + t(A))/2$.

**Details**

For each cardinality $k$ (with $k$ ranging from $k_{\text{min}}$ to $k_{\text{max}}$), an initial population of $\text{popsize}$ $k$-variable subsets is randomly selected from a full set of $p$ variables. In each iteration, $\text{popsize}/2$ couples are formed from among the population and each couple generates a child (a new $k$-variable subset) which inherits properties of its parents (specifically, it inherits all variables common to both parents and a random selection of variables in the symmetric difference of its parents’ genetic makeup). Each offspring may optionally undergo a mutation (in the form of a local improvement algorithm – see function `improve`), with a user-specified probability. The parents and offspring are ranked according to their criterion value, and the best $\text{popsize}$ of these $k$-subsets will make up the next generation, which is used as the current population in the subsequent iteration.

The stopping rule for the algorithm is the number of generations ($\text{nger}$).

Optionally, the best $k$-variable subset produced by the Genetic Algorithm may be passed as input to a restricted local improvement algorithm, for possible further improvement (see function `improve`).

The user may force variables to be included and/or excluded from the $k$-subsets, and may specify an initial population.

For each cardinality $k$, the total number of calls to the procedure which computes the criterion values is $\text{popsize} + \text{nger} \times \text{popsize}/2$. These calls are the dominant computational effort in each iteration of the algorithm.

In order to improve computation times, the bulk of computations are carried out by a Fortran routine. Further details about the Genetic Algorithm can be found in Reference 1 and in the comments to the Fortran code (in the src subdirectory for this package). For datasets with a very large number of variables (currently $p > 400$), it is necessary to set the `force` argument to TRUE for the function to run, but this may cause a session crash if there is not enough memory available.
The function checks for ill-conditioning of the input matrix (specifically, it checks whether the ratio of the input matrix’s smallest and largest eigenvalues is less than tolval). For an ill-conditioned input matrix, the search is restricted to its well-conditioned subsets. The function trim.matrix may be used to obtain a well-conditioned input matrix.

In a general descriptive (Principal Components Analysis) setting, the three criteria Rm, Rv and Gcd can be used to select good k-variable subsets. Arguments H and r are not used in this context. See references [1] and [2] and the Examples for a more detailed discussion.

In the setting of a multivariate linear model, \(X = A\Psi + U\), criteria Ccr12, Tau2, Xi2 and Zeta2 can be used to select subsets according to their contribution to an effect characterized by the violation of a reference hypothesis, \(C\Psi = 0\) (see reference [3] for further details). In this setting, arguments mat and H should be set respectively to the usual Total (Hypothesis + Error) and Hypothesis, Sum of Squares and Cross-Products (SSCP) matrices. Argument r should be set to the expected rank of H. Currently, for reasons of computational efficiency, criterion Ccr12 is available only when \(r \leq 3\). Particular cases in this setting include Linear Discriminant Analysis (LDA), Linear Regression Analysis (LRA), Canonical Correlation Analysis (CCA) with one set of variables fixed and several extensions of these and other classical multivariate methodologies.

In the setting of a generalized linear model, criterion Wald can be used to select subsets according to the (lack of) significance of the discarded variables, as measured by the respective Wald’s statistic (see reference [4] for further details). In this setting arguments mat and H should be set respectively to FI and FI \(\%\% b \%\% t(b) \%\% FI\), where b is a column vector of variable coefficient estimates and FI is an estimate of the corresponding Fisher information matrix.

The auxiliary functions lmHmat, ldaHmat glhHmat and glmHmat are provided to automatically create the matrices mat and H in all the cases considered.

Value

A list with five items:

- **subsets** is a popsize x kmax x length(kmin:kmax) 3-dimensional array, giving for each cardinality (dimension 3) and each subset in the final population (dimension 1) the list of variables (referenced by their row/column numbers in matrix mat) in the subset (dimension 2). (For cardinalities smaller than kmax, the extra final positions are set to zero).

- **values** is a popsize x length(kmin:kmax) matrix, giving for each cardinality (columns), the (ordered) criterion values of the popsize (rows) subsets in the final generation.

- **bestvalues** is a length(kmin:kmax) vector giving the best values of the criterion obtained for each cardinality. If improvement is TRUE, these values result from the final restricted local search algorithm (and may therefore exceed the largest value for that cardinality in values).

- **bestsets** is a length(kmin:kmax) x kmax matrix, giving, for each cardinality (rows), the variables (referenced by their row/column numbers in matrix mat) in the best k-subset that was found.

- **call** is the function call which generated the output.
References


See Also

rm.coef, rv.coef, gcd.coef, tau2.coef, xi2.coef, zeta2.coef, ccr12.coef, genetic, anneal, eleaps, trim.matrix, lmmHmat, ldaHmat, glhHmat, glmHmat.

Examples

```r
## 1) For illustration of use, a small data set with very few iterations
## of the algorithm. Escoufier 's 'RV' criterion is used to select variable
## subsets of size 3 and 4.

data(swiss)
genetic(cor(swiss),3,4,popsize=10,nger=5,criterion="Rv")

## For cardinality k=
## 4
## there is not enough genetic diversity in generation number
## 3
## for acceptable levels of consanguinity (couples differing by at least 2 genes).
## Try reducing the maximum acceptable number of clones (maxclone) or
## increasing the population size (popsize)
## Best criterion value found so far:
## 0.9557145
##$subsets
## , , Card.3
## Var.1 Var.2 Var.3 Var.4
## Solution 1 1 2 3 0
## Solution 2 1 2 3 0
## Solution 3 1 2 3 0
## Solution 4 3 4 6 0
## Solution 5 3 4 6 0
## Solution 6 3 4 5 0
## Solution 7 3 4 5 0
```
## Solution 8 1 3 6 0
## Solution 9 1 3 6 0
## Solution 10 1 3 6 0
#
## , , Card.4
##
## Var.1 Var.2 Var.3 Var.4
## Solution 1 2 4 5 6
## Solution 2 1 2 5 6
## Solution 3 1 2 3 5
## Solution 4 1 2 4 5
## Solution 5 1 2 4 5
## Solution 6 1 4 5 6
## Solution 7 1 4 5 6
## Solution 8 1 4 5 6
## Solution 9 1 3 4 5
## Solution 10 1 3 4 5
#
## $values
card.3 card.4
## Solution 1 0.9141995 0.9557145
## Solution 2 0.9141995 0.9485699
## Solution 3 0.9141995 0.9455508
## Solution 4 0.9034868 0.9433203
## Solution 5 0.9034868 0.9433203
## Solution 6 0.9020271 0.9428967
## Solution 7 0.9020271 0.9428967
## Solution 8 0.8988192 0.9428967
## Solution 9 0.8988192 0.9357982
## Solution 10 0.8988192 0.9357982
#
## $bestvalues
## Card.3 Card.4
## 0.9141995 0.9557145
#
## $bestsets
## Var.1 Var.2 Var.3 Var.4
## Card.3 1 2 3 0
## Card.4 2 4 5 6
#
## $call
## genetic(mat = cor(swiss), kmin = 3, kmax = 4, popsize = 10, nger = 5,
## criterion = "Rv")

# 2) An example of subset selection in the context of Multiple Linear Regression. Variable 5 (average car price) in the Cars93 MASS library data set is regressed on 13 other variables. The six-variable subsets
## of linear predictors are chosen using the "CCR1_2" criterion which, in the case of a Linear Regression, is merely the standard Coefficient of Determination, $R^2$ (as are the other three criteria for the multivariate linear hypothesis, "XI_2", "TAU_2" and "ZETA_2").

library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,5])

names(Cars93[,5,drop=FALSE])
## [1] "Price"

colnames(CarsHmat)
## [1] "MPG.city"  "MPG.highway"  "EngineSize"
## [4] "Horsepower"  "RPM"  "Rev.per.mile"
## [7] "Fuel.tank.capacity"  "Passengers"  "Length"
## [10] "Wheelbase"  "Width"  "Turn.circle"
## [13] "Weight"

genetic(CarsHmat$mat, kmin=6, H=CarsHmat$H, r=1, crit="CCR12")

## (Partial results only)
##
## $subsets
##
## Solution 1   Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 2   4   5   9   10   11   12
## Solution 3   4   5   9   10   11   12
## Solution 4   4   5   9   10   11   12
## Solution 5   4   5   9   10   11   12
## Solution 6   4   5   9   10   11   12
## Solution 7   4   5   8   10   11   12
##
## (...)
##
## Solution 94  1   4   5   6   10   11
## Solution 95  1   4   5   6   10   11
## Solution 96  1   4   5   6   10   11
## Solution 97  1   4   5   6   10   11
## Solution 98  1   4   5   6   10   11
## Solution 99  1   4   5   6   10   11
## Solution 100 1   4   5   6   10   11
##
## $values
##
## Solution 1  Solution 2  Solution 3  Solution 4  Solution 5  Solution 6
## 0.7310150  0.7310150  0.7310150  0.7310150  0.7310150  0.7310150
## Solution 7  Solution 8  Solution 9  Solution 10  Solution 11  Solution 12
## 0.7310150  0.7271056  0.7271056  0.7271056  0.7271056  0.7271056
## Solution 13  Solution 14  Solution 15  Solution 16  Solution 17  Solution 18
3) An example of subset selection in the context of a Canonical Correlation Analysis. Two groups of variables within the Cars93 MASS library data set are compared. The goal is to select 4- to 6-variable subsets of the 13-variable 'X' group that are optimal in terms of preserving the canonical correlations, according to the "ZETA_2" criterion (Warning: the 3-variable 'Y' group is kept intact; subset selection is carried out in the 'X' group only). The 'tolsym' parameter is used to relax the symmetry requirements on the effect matrix H which, for numerical reasons, is slightly asymmetric. Since corresponding off-diagonal entries of matrix H are different, but by less than tolsym, H is replaced by its symmetric part: (H+t(H))/2.

library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,4:6])
names(Cars93[,4:6])
colnames(CarsHmat$mat)
## [1] "MPG.city" "MPG.highway" "EngineSize"
## [4] "Horsepower" "RPM" "Rev.per.mile"
## [7] "Fuel.tank.capacity" "Passengers" "Length"
## [10] "Wheelbase" "Width" "Turn.circle"
## [13] "Weight"
genetic(CarsHmat$mat, kmin=5, kmax=6, H=CarsHmat$H, r=3, crit="zeta2", tolsym=1e-9)

## (PARTIAL RESULTS ONLY)
##
## $subsets
##
## |   | Var.1 | Var.2 | Var.3 | Var.4 | Var.5 | Var.6 |
##---|-------|-------|-------|-------|-------|-------|
## Solution 1 | 4     | 5     | 9     | 10    | 11    |   0   |
## Solution 2 | 4     | 5     | 9     | 10    | 11    |   0   |
## Solution 3 | 4     | 5     | 9     | 10    | 11    |   0   |
## Solution 4 | 4     | 5     | 9     | 10    | 11    |   0   |
## Solution 5 | 4     | 5     | 9     | 10    | 11    |   0   |
## Solution 6 | 4     | 5     | 9     | 10    | 11    |   0   |
## Solution 7 | 4     | 5     | 9     | 10    | 11    |   0   |
## Solution 8 | 3     | 4     | 9     | 10    | 11    |   0   |
## Solution 9 | 3     | 4     | 9     | 10    | 11    |   0   |
## Solution 10| 3     | 4     | 9     | 10    | 11    |   0   |
## (...)
##
## $values
##
## |   | card.5 | card.6 |
##---|-------|-------|
## Solution 1 | 0.5018922 | 0.5168627 |
## Solution 2 | 0.5018922 | 0.5168627 |
## Solution 3 | 0.5018922 | 0.5168627 |
## Solution 4 | 0.5018922 | 0.5168627 |
## Solution 5 | 0.5018922 | 0.5168627 |
## Solution 6 | 0.5018922 | 0.5168627 |
## Solution 7 | 0.5018922 | 0.5096500 |
## Solution 8 | 0.4966191 | 0.5096500 |
## Solution 9 | 0.4966191 | 0.5096500 |
## Solution 10| 0.4966191 | 0.5096500 |
## (...)

## Solution 87 0.4893824 0.5038649
## Solution 88 0.4893824 0.5038649
## Solution 89 0.4893824 0.5038649
## Solution 90 0.4893824 0.5035489
## Solution 91 0.4893824 0.5035489
## Solution 92 0.4893824 0.5035489
## Solution 93 0.4893824 0.5035489
## Solution 94 0.4893824 0.5035489
## Solution 95 0.4893824 0.5035489
## Solution 96 0.4893824 0.5035489
## Solution 97 0.4890986 0.5035386
## Solution 98 0.4890986 0.5035386
## Solution 99 0.4890986 0.5035386
## Solution 100 0.4890986 0.5035386
##
## $bestvalues
## Card.5 Card.6
## 0.5018922 0.5168627
##
## $bestsets
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Card.5 4 5 9 10 11 0
## Card.6 4 5 9 10 11 12
##
## $call
## genetic(mat = CarsHmat$mat, kmin = 5, kmax = 6, criterion = "zeta2",
## H = CarsHmat$H, r = 3, tolsym = 1e-09)
##
## Warning message:
##
## The effect description matrix (H) supplied was slightly asymmetric:
## symmetric entries differed by up to 3.63797880709171e-12.
## (less than the 'tolsym' parameter).
## The H matrix has been replaced by its symmetric part.
## in: validnovcrit(mat, criterion, H, r, p, tolval, tolsym)
##
## The selected best variable subsets

colnames(CarsHmat$mat)[c(4,5,9,10,11)]

## [1] "Horsepower" "RPM" "Length" "Wheelbase" "Width"

colnames(CarsHmat$mat)[c(4,5,9,10,11,12)]

## [1] "Horsepower" "RPM" "Length" "Wheelbase" "Width"
## [6] "Turn.circle"

# --------------------------------------------------------------------
Total and Effect Deviation Matrices for General Linear Hypothesis

Description

Computes total and effect matrices of Sums of Squares and Cross-Product (SSCP) deviations for a general multivariate effect characterized by the violation of a linear hypothesis. These matrices may be used as input to the variable selection search routines `anneal`, `genetic improve` or `eleaps`.

Usage

```r
## Default S3 method:
glhHmat(x, A, C, ...)
## S3 method for class 'data.frame'
glhHmat(x, A, C, ...)
## S3 method for class 'formula'
glhHmat(formula, C, data = NULL, ...)
```

Arguments

- `x` A matrix or data frame containing the variables for which the SSCP matrix is to be computed.
- `A` A matrix or data frame containing a design matrix specifying a linear model in which `x` is the response.
- `C` A matrix or vector containing the coefficients of the reference hypothesis.
- `formula` A formula of the form `x ~ A1 + A2 + ...` That is, the response is the set of variables whose subsets are to be compared and the right hand side specifies the columns of the design matrix.
- `data` Data frame from which variables specified in `formula` are preferentially to be taken.
- `...` Further arguments for the method.

Details

Consider a multivariate linear model \( x = A\Psi + U \) and a reference hypothesis \( H_0 : C\Psi = 0 \), with \( \Psi \) being a matrix of unknown parameters and \( C \) a known coefficient matrix with rank \( r \). It is well known that, under classical Gaussian assumptions, \( H_0 \) can be tested by several increasing functions of the \( r \) positive eigenvalues of a product \( T^{-1}H \), where \( T \) and \( H \) are total and effect matrices of SSCP deviations associated with \( H_0 \). Furthermore, whether or not the classical assumptions hold, the same eigenvalues can be used to define descriptive indices that measure an "effect" characterized by the violation of \( H_0 \) (see reference [1] for further details). Those SSCP matrices are given by \( T = x'(I - P_\omega)x \) and \( H = x'(P_\Omega - P_\omega)x \), where \( I \) is an identity matrix and \( P_\Omega = A(A'\tilde{A})^{-1}A' \),
\[ P_c = A(A'A)^{-} A' - A(A'A)^{-} C'[C(A'A)^{-} C']^{-} C(A'A)^{-} A' \]

are projection matrices on the spaces spanned by the columns of \( A \) (space \( \Omega \)) and by the linear combinations of these columns that satisfy the reference hypothesis (space \( \omega \)). In these formulae \( M' \) denotes the transpose of \( M \) and \( M^{-} \) a generalized inverse. \texttt{glhHmat} computes the \( T \) and \( H \) matrices which then can be used as input to the search routines \texttt{anneal}, \texttt{genetic improve} and \texttt{eleaps} that try to select subsets of \( x \) according to their contribution to the violation of \( H_0 \).

**Value**

A list with four items:

- \texttt{mat} \quad The total SSCP matrix
- \texttt{H} \quad The effect SSCP matrix
- \texttt{r} \quad The expected rank of the H matrix which equals the rank of \( C \). The true rank of \( H \) can be different from \( r \) if the \( x \) variables are linearly dependent.
- \texttt{call} \quad The function call which generated the output.

**References**


**See Also**

\texttt{anneal}, \texttt{genetic}, \texttt{improve}, \texttt{eleaps}, \texttt{lmHmat}, \texttt{ldaHmat}.

**Examples**

```r
## The following examples create T and H matrices for different analysis
## of the MASS data set "crabs". This data records physical measurements
## on 200 specimens of Leptograpsus variegatus crabs observed on the shores
## of Western Australia. The crabs are classified by two factors, sex and sp
## (crab species as defined by its colour: blue or orange), with two levels
## each. The measurement variables include the carapace length (CL),
## the carapace width (CW), the size of the frontal lobe (FL) and the size of
## the rear width (RW). In the analysis provided, we assume that there is
## an interest in comparing the subsets of these variables measured in their
## original and logarithmic scales.

library(MASS)
data(crabs)
lFL <- log(crabs$FL)
lRW <- log(crabs$RW)
lCL <- log(crabs$CL)
lCW <- log(crabs$CW)
```
# 1) Create the T and H matrices associated with a linear discriminant analysis on the groups defined by the sp factor. This call is equivalent to ldaHmat(sp ~ FL + RW + CL + CW + lFL + lRW + lCL + lCW, crabs)

Hmat1 <- glhHmat(cbind(FL,RW,CL,CW,lFL,lRW,lCL,lCW) ~ sp, c(0,1), crabs)
Hmat1

###$mat
```r
# FL RW CL CW lFL lRW lCL
## FL 2431.2422 1623.4509 4846.9787 5283.6093 162.718609 133.360397 158.865134
## RW 1623.4509 1317.7935 3254.5776 3629.6883 109.877182 107.287243 108.335721
## CL 4846.9787 3254.5776 10085.3040 11096.5141 326.243285 269.564742 330.912570
## CW 5283.6093 3629.6883 11096.5141 12331.5680 356.317934 300.786770 364.620761
## lRW 133.3604 107.2872 269.5647 300.7868 9.188391 8.906350 9.130692
## lCW 152.7872 106.4277 321.0253 357.0051 10.503303 8.970570 10.765175
```

###$H
```r
# FL RW CL CW lFL lRW lCL
## FL 466.34580 247.526700 625.30650 518.41650 30.7408809 19.4543286 20.5494907
## CL 625.30650 331.89975 838.45125 695.12625 41.2193540 26.0856066 27.5540813
## CW 518.41650 275.164750 695.12625 576.30125 34.1733106 21.6265286 22.8439819
## lFL 30.74088 16.316623 41.21935 34.17331 2.0263971 1.2824024 1.3549545
## lRW 19.45432 10.325951 26.08561 21.62653 1.2824024 0.8115664 0.8572531
## lCL 20.54949 10.907244 27.55408 22.84398 1.3549545 0.8572531 0.9055117
## lCW 15.16136 8.047335 20.32933 16.85423 0.9994161 0.6324790 0.6680840
```

###$r
```
[1] 1
```

###$call
```
# glhHmat.formula(formula = cbind(FL, RW, CL, CW, lFL, lRW, lCL, lCW, crabs)
```
## glhHmat

```r
## 1CW) ~ sp, C = c(0, 1), data = crabs)

# 2) Create the T and H matrices associated with an analysis
# of the interactions between the sp and sex factors
Hmat2 <- g lhHmat(cbind(FL,RW,CL,CW,lFL,lRW,lCL,lCW) ~ sp*sex,c(0,0,0,1),crabs)
Hmat2

###$mat

<table>
<thead>
<tr>
<th></th>
<th>FL</th>
<th>RW</th>
<th>CL</th>
<th>CW</th>
<th>lFL</th>
<th>lRW</th>
<th>lCL</th>
</tr>
</thead>
<tbody>
<tr>
<td>FL</td>
<td>1960.3362</td>
<td>1398.5289</td>
<td>4199.1581</td>
<td>4747.5409</td>
<td>131.6518</td>
<td>115.607172</td>
<td>137.663744</td>
</tr>
<tr>
<td>RW</td>
<td>1398.5289</td>
<td>1074.36105</td>
<td>3034.2793</td>
<td>3442.0233</td>
<td>95.176151</td>
<td>88.529040</td>
<td>100.659912</td>
</tr>
<tr>
<td>CL</td>
<td>4199.1581</td>
<td>3034.27925</td>
<td>9135.6987</td>
<td>10314.2389</td>
<td>283.414814</td>
<td>251.877591</td>
<td>300.140005</td>
</tr>
<tr>
<td>CW</td>
<td>4747.5409</td>
<td>3442.02325</td>
<td>10314.2389</td>
<td>11686.9387</td>
<td>320.883015</td>
<td>285.744945</td>
<td>339.253367</td>
</tr>
<tr>
<td>lFL</td>
<td>131.6518</td>
<td>95.17615</td>
<td>283.4148</td>
<td>320.8830</td>
<td>9.065041</td>
<td>8.027569</td>
<td>9.509543</td>
</tr>
<tr>
<td>lRW</td>
<td>115.6072</td>
<td>88.52904</td>
<td>251.8776</td>
<td>285.7449</td>
<td>8.027569</td>
<td>7.460222</td>
<td>8.516618</td>
</tr>
<tr>
<td>lCL</td>
<td>137.6637</td>
<td>100.65991</td>
<td>300.1400</td>
<td>339.2534</td>
<td>9.509543</td>
<td>8.516618</td>
<td>10.090003</td>
</tr>
<tr>
<td>lCW</td>
<td>137.205863</td>
<td>100.462028</td>
<td>298.622747</td>
<td>338.525352</td>
<td>9.473873</td>
<td>8.494741</td>
<td>10.037059</td>
</tr>
</tbody>
</table>

###$H

<table>
<thead>
<tr>
<th></th>
<th>FL</th>
<th>RW</th>
<th>CL</th>
<th>CW</th>
<th>lFL</th>
<th>lRW</th>
<th>lCL</th>
</tr>
</thead>
<tbody>
<tr>
<td>FL</td>
<td>80.645000</td>
<td>68.389500</td>
<td>153.73350</td>
<td>191.57950</td>
<td>5.4708199</td>
<td>5.1596883</td>
<td>5.2140868</td>
</tr>
<tr>
<td>RW</td>
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<td>57.996450</td>
<td>130.37085</td>
<td>162.46545</td>
<td>4.6394276</td>
<td>4.3755782</td>
<td>4.4217098</td>
</tr>
<tr>
<td>CL</td>
<td>153.73350</td>
<td>130.37085</td>
<td>293.06205</td>
<td>365.20785</td>
<td>10.4290197</td>
<td>9.83509098</td>
<td>9.9396095</td>
</tr>
<tr>
<td>CW</td>
<td>191.57950</td>
<td>162.46545</td>
<td>365.20785</td>
<td>455.11445</td>
<td>12.9964281</td>
<td>12.2573068</td>
<td>12.3865353</td>
</tr>
<tr>
<td>lFL</td>
<td>5.470820</td>
<td>4.639428</td>
<td>10.42902</td>
<td>12.99643</td>
<td>0.3711311</td>
<td>0.3500245</td>
<td>0.3537148</td>
</tr>
<tr>
<td>lRW</td>
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<td>4.375578</td>
<td>9.83591</td>
<td>12.25731</td>
<td>0.3500245</td>
<td>0.3301182</td>
<td>0.3335986</td>
</tr>
<tr>
<td>lCL</td>
<td>5.214087</td>
<td>4.421710</td>
<td>9.93961</td>
<td>12.38654</td>
<td>0.3537148</td>
<td>0.3335986</td>
<td>0.3371158</td>
</tr>
<tr>
<td>lCW</td>
<td>5.584150</td>
<td>4.735535</td>
<td>10.64506</td>
<td>13.26565</td>
<td>0.3788193</td>
<td>0.3572754</td>
<td>0.3610421</td>
</tr>
</tbody>
</table>

###$r

r [1] 1

###$call
```
```
## glhHmat.formula(formula = cbind(FL, RW, CL, CW, lFL, lRW, lCL,
## 1CW) ~ sp * sex, C = c(0, 0, 0, 1), data = crabs)

## 3) Create the T and H matrices associated with an analysis
## of the effect of the sp factor after controlling for sex

C <- matrix(0.,2,4)
C
## [1,] 0 0 1 0
## [2,] 0 0 0 1

Hmat3 <- glhHmat(cbind(FL,RW,CL,CW,lFL,lRW,lCL,lCW) ~ sp*sex,C,crabs)
Hmat3
```

### $mat
```
## FL  RW  CL  CW  lFL  lRW  1CW
## FL  1964.8964  1375.9242  4221.6722  4765.1928  131.977728  113.906076  138.315643
## RW  1375.9242  1186.41150  2922.6779  3354.5236  93.560559  96.961292  97.428477
## CL  4221.6722  2922.67790  9246.8527 10401.3878 285.023931 243.479136 303.358489
## CW  4765.1928 3354.52360 10401.3878 11755.2667 322.144623 279.160241 341.776779
## lFL 131.9777 93.56056 285.0239 322.1446 9.088336 7.905989 9.556135
## lRW 113.9061 96.96129 243.4791 279.1602 7.905989 8.094783 8.273439
## lCL 138.3156 97.42848 303.3585 341.7768 9.556135 8.273439 10.183194
## lCW 137.6258 98.38041 300.6960 340.1509 9.503886 8.338091 10.097091
## lCW 137.625801
## RW 98.380414
## CL 300.696018
## CW 340.150874
## lFL 9.503886
## lRW 8.338091
## lCL 10.097091
## lCW 10.050426
```

### $H
```
## FL  RW  CL  CW  lFL  lRW
## FL  85.205200  45.784800  176.247600  209.231400  5.796744  3.45859277
## RW  45.784800  176.247600  18.769500  74.965800  3.0238356 12.80782993
## CL 176.247600  18.769500 404.216100  452.356800 12.0381364 1.43745463
## CW 209.231400  74.965800  452.356800 523.442500 14.2580360 5.67260253
## lFL  5.796744 3.023836 12.807829 14.258036 0.3944254 0.22844463
## lRW 3.458593 12.807830 1.437455 5.672603 0.2284446 0.96467943
## lCL 5.865986 1.190274 13.158933 14.909948 0.4003070 0.09041999
## lCW 6.004088 2.653921 12.718332 14.891177 0.488329 0.20062548
## lCW 5.86598627 6.004088
## RW 1.19027431 2.653921
## CL 13.15893339 12.7183319
## CW 14.90994753 14.8911765
## lFL 0.40030784 0.488329
```
glmHmat

## glmHmat

Input matrices for subselect search routines in generalized linear models

Description

glmHmat uses a glm object (fitdglmmodel) to build an estimate of Fisher’s Information (FI) matrix together with an auxiliarly rank-one positive-definite matrix (H), such that the positive eigenvalue of \( FI^{-1} H \) equals the value of Wald’s statistic for testing the global significance of fitdglmmodel. These matrices may be used as input to the variable selection search routines `anneal`, `genetic`, `improve` or `eleaps`, using the minimization of Wald’s statistic as criterion for discarding variables.

Usage

```r
### S3 method for class 'glm'
glmHmat(fitdglmmodel,...)
```

Arguments

- `fitdglmmodel`: A glm object containing the estimates, and respective covariance matrix, of a generalized linear model.
- `...`: further arguments for the method.

Details

Variable selection in the context of generalized linear models is typically based on the minimization of statistics that test the significance of excluded variables. In particular, the likelihood ratio, Wald’s, Rao’s and some adaptations of such statistics, are often proposed as comparison criteria for variable subsets of the same dimensionality. All these statistics are asymptotically equivalent and can be converted into information criteria, like the AIC, that are also able to compare subsets of different dimensionalities (see references [1] and [2] for further details).

Among these criteria, Wald’s statistic has some computational advantages because it can always be derived from the same (concerning the full model) maximum likelihood and Fisher information.
estimates. In particular, if $W_{allv}$ is the value of the Wald statistic testing the significance of the full covariate vector, $b$ and $FI$ are coefficient and Fisher information estimates and $H$ is an auxiliary rank-one matrix given by $H = FI \times b \times t(b) \times FI$, it follows that the value of Wald’s statistic for the excluded variables ($W_{excv}$) in a given subset is given by

$$W_{excv} = W_{allv} - tr(FI^{-1}_{indices} H_{indices}),$$

where $FI_{indices}$ and $H_{indices}$ are the portions of the $FI$ and $H$ matrices associated with the selected variables.

glmHmat retrieves the values of the $FI$ and $H$ matrices from a glm object. These matrices may then be used as input to the search functions `anneal`, `genetic`, `improve` and `eleaps`.

Value

A list with four items:

- mat: An estimate (FI) of Fisher’s information matrix for the full model variable-coefficient estimates
- $H$: A product of the form $(FI \times b \times t(b) \times FI)$ where $b$ is a vector of variable-coefficient estimates
- $r$: The rank of the $H$ matrix. Always set to one in glmHmat.
- call: The function call which generated the output.

References


See Also

`anneal`, `genetic`, `improve`, `eleaps`, `glm`.

Examples

```r
## An example of variable selection in the context of binary response models. We consider the last 100 observations of the iris data set (versicolor an virginica species) and try to find the best variable subsets for models that take species as the response variable.

data(iris)
iris2sp <- iris[iris$Species != "setosa",]
```
# Create the input matrices for the search routines in a logistic regression model

```r
modelfit <- glm(Species ~ Sepal.Length + Sepal.Width + Petal.Length + Petal.Width, iris2sp, family=binomial)
Hmat <- glmHmat(modelfit)
Hmat
## $mat
## Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length 0.28340358 0.03263437 0.09552821 -0.01779067
## Sepal.Width 0.03263437 0.13941541 0.01086596 0.04759284
## Petal.Length 0.09552821 0.01086596 0.08847655 -0.01853044
## Petal.Width -0.01779067 0.04759284 -0.01853044 0.03258730
## $H
## Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length 0.11643732 0.013349227 -0.063924853 -0.050181400
## Sepal.Width 0.01334923 0.001530453 -0.007328813 -0.005753163
## Petal.Length -0.06392485 -0.007328813 0.035095164 0.027549918
## Petal.Width -0.05018140 -0.005753163 0.027549918 0.021626854
## $r
## [1] 1
## $call
glmHmat(fitdglmmodel = modelfit)
```

# Search for the 3 best variable subsets of each dimensionality by an exhaustive search

```r
eleaps(Hmat$mat, H=Hmat$H, r=1, criterion="Wald", nsol=3)
```

### $subsets

#### , , Card.1

<table>
<thead>
<tr>
<th>Var.1</th>
<th>Var.2</th>
<th>Var.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solution 1</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>Solution 2</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Solution 3</td>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

#### , , Card.2

<table>
<thead>
<tr>
<th>Var.1</th>
<th>Var.2</th>
<th>Var.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solution 1</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Solution 2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Solution 3</td>
<td>2</td>
<td>4</td>
</tr>
</tbody>
</table>

#### , , Card.3

<table>
<thead>
<tr>
<th>Var.1</th>
<th>Var.2</th>
<th>Var.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solution 1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Solution 2</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Solution 3</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>
## $values
## | card.1 | card.2 | card.3 |
## |--------|--------|--------|
## Solution 1 | 4.894554 | 3.522885 | 1.060121 |
## Solution 2 | 5.147360 | 3.952538 | 2.224335 |
## Solution 3 | 5.161553 | 3.972410 | 3.522879 |

## $bestvalues
## | Card.1 | Card.2 | Card.3 |
## |--------|--------|--------|
## | 4.894554 | 3.522885 | 1.060121 |

## $bestsets
## | Var.1 | Var.2 | Var.3 |
## |-------|-------|-------|
## | Card.1 | 4 | 0 | 0 |
## | Card.2 | 1 | 3 | 0 |
## | Card.3 | 2 | 3 | 4 |

## $call
## eleaps(mat = Hmat$mat, nsol = 3, criterion = "Wald", H = Hmat$H, 
## r = 1)

It should be stressed that, unlike other criteria in the 
subselect package, the Wald criterion is not bounded above by 
1 and is a decreasing function of subset quality, so that the 
3-variable subsets do, in fact, perform better than their smaller-sized 
counterparts.

> proc.time()
> [1] 0.680 0.064 0.736 0.000 0.000

---

**improve**

**Restricted Local Improvement search for an optimal k-variable subset**

**Description**

Given a set of variables, a Restricted Local Improvement algorithm seeks a k-variable subset which is optimal, as a surrogate for the whole set, with respect to a given criterion.

**Usage**

```r
improve( mat, kmin, kmax = kmin, nsol = 1, exclude = NULL, 
include = NULL, setseed = FALSE, criterion = "default", pcindices="first_k", 
initialsol = NULL, force = FALSE, H=NULL, r=0, 
tolval=1000*.Machine$double.eps,tolsym=1000*.Machine$double.eps)
```
Arguments

mat
a covariance/correlation, information or sums of squares and products matrix of the variables from which the k-subset is to be selected. See the Details section below.

kmin
the cardinality of the smallest subset that is wanted.

kmax
the cardinality of the largest subset that is wanted.

nsol
the number of different subsets (runs of the algorithm) wanted.

exclude
a vector of variables (referenced by their row/column numbers in matrix mat) that are to be forcibly excluded from the subsets.

include
a vector of variables (referenced by their row/column numbers in matrix mat) that are to be forcibly included from the subsets.

setseed
logical variable indicating whether to fix an initial seed for the random number generator, which will be re-used in future calls to this function whenever setseed is again set to TRUE.

criterion
Character variable, which indicates which criterion is to be used in judging the quality of the subsets. Currently, the "Rm", "Rv", "Gcd", "Tau2", "Xi2", "Zeta2", "ccr12" and "Wald" criteria are supported (see the Details section, the References and the links rm.coef, rv.coef, gcd.coef, tau2.coef, xi2.coef, zeta2.coef and ccr12.coef for further details). The default criterion is "Rm" if parameter r is zero (exploratory and PCA problems), "Wald" if r is equal to one and mat has a "FisherI" attribute set to TRUE (generalized linear models), and "Tau2" otherwise (multivariate linear model framework).

pcindices
either a vector of ranks of Principal Components that are to be used for comparison with the k-variable subsets (for the Gcd criterion only, see gcd.coef) or the default text first_k. The latter will associate PCs 1 to k with each cardinality k that has been requested by the user.

initialsol
vector, matrix or 3-d array of initial solutions for the restricted local improvement search. If a single cardinality is required, initialsol may be a vector of length k (accepted even if nsol > 1, in which case it is used as the initial solution for all nsol final solutions that are requested with a warning that the same initial solution necessarily produces the same final solution); a 1 x k matrix (as produced by the $bestsets output value of the algorithm functions anneal, genetic, or improve), or a 1 x k x 1 array (as produced by the $subsets output value), in which case it will be treated as the above k-vector; or an nsol x k matrix, or nsol x k x 1 3-d array, in which case each row (dimension 1) will be used as the initial solution for each of the nsol final solutions requested. If more than one cardinality is requested, initialsol can be a length(kmin:kmax) x kmax matrix (as produced by the $bestsets option of the algorithm functions) (even if nsol > 1, in which case each row will be replicated to produced the initial solution for all nsol final solutions requested in each cardinality, with a warning that a single initial solution necessarily produces identical final solutions), or a nsol x kmax x length(kmin:kmax) 3-d array (as produced by the $subsets output option), in which case each row (dimension 1) is interpreted as a different initial solution.

If the exclude and/or include options are used, initialsol must also respect those requirements.
force

a logical variable indicating whether, for large data sets (currently \( p > 400 \)) the algorithm should proceed anyways, regardless of possible memory problems which may crash the R session.

\( H \)

Effect description matrix. Not used with the Rm, Rv or Gcd criteria, hence the NULL default value. See the Details section below.

\( r \)

Expected rank of the effects (\( H \)) matrix. Not used with the Rm, Rv or Gcd criteria. See the Details section below.

tolval

the tolerance level for the reciprocal of the 2-norm condition number of the correlation/covariance matrix, i.e., for the ratio of the smallest to the largest eigenvalue of the input matrix. Matrices with a reciprocal of the condition number smaller than toval will activate a restricted-search for well conditioned subsets.

tolsym

the tolerance level for symmetry of the covariance/correlation/total matrix and for the effects (\( H \)) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes \((A + t(A))/2\).

Details

An initial k-variable subset (for \( k \) ranging from \( k_{\text{min}} \) to \( k_{\text{max}} \)) of a full set of \( p \) variables is randomly selected and the variables not belonging to this subset are placed in a queue. The possibility of replacing a variable in the current k-subset with a variable from the queue is then explored. More precisely, a variable is selected, removed from the queue, and the k values of the criterion which would result from swapping this selected variable with each variable in the current subset are computed. If the best of these values improves the current criterion value, the current subset is updated accordingly. In this case, the variable which leaves the subset is added to the queue, but only if it has not previously been in the queue (i.e., no variable can enter the queue twice). The algorithm proceeds until the queue is emptied.

The user may force variables to be included and/or excluded from the k-subsets, and may specify initial solutions.

For each cardinality \( k \), the total number of calls to the procedure which computes the criterion values is \( O(n_{\text{sol}} \times k \times p) \). These calls are the dominant computational effort in each iteration of the algorithm.

In order to improve computation times, the bulk of computations are carried out in a Fortran routine. Further details about the algorithm can be found in Reference 1 and in the comments to the Fortran code (in the src subdirectory for this package). For datasets with a very large number of variables (currently \( p > 400 \)), it is necessary to set the force argument to TRUE for the function to run, but this may cause a session crash if there is not enough memory available.

The function checks for ill-conditioning of the input matrix (specifically, it checks whether the ratio of the input matrix’s smallest and largest eigenvalues is less than toval). For an ill-conditioned input matrix, the search is restricted to its well-conditioned subsets. The function trim.matrix may be used to obtain a well-conditioned input matrix.

In a general descriptive (Principal Components Analysis) setting, the three criteria Rm, Rv and Gcd can be used to select good k-variable subsets. Arguments \( H \) and \( r \) are not used in this context. See references [1] and [2] and the Examples for a more detailed discussion.
In the setting of a multivariate linear model, $X = A\Psi + U$, criteria Ccr12, Tau2, Xi2 and Zeta2 can be used to select subsets according to their contribution to an effect characterized by the violation of a reference hypothesis, $C\Psi = 0$ (see reference [3] for further details). In this setting, arguments `mat` and `H` should be set respectively to the usual Total (Hypothesis + Error) and Hypothesis, Sum of Squares and Cross-Products (SSCP) matrices. Argument `r` should be set to the expected rank of `H`. Currently, for reasons of computational efficiency, criterion Ccr12 is available only when $r \leq 3$. Particular cases in this setting include Linear Discriminant Analysis (LDA), Linear Regression Analysis (LRA), Canonical Correlation Analysis (CCA) with one set of variables fixed and several extensions of these and other classical multivariate methodologies.

In the setting of a generalized linear model, criterion Wald can be used to select subsets according to the (lack of) significance of the discarded variables, as measured by the respective Wald's statistic (see reference [4] for further details). In this setting arguments `mat` and `H` should be set respectively to $FI$ and $FI \%*% b \%*% t(b) \%*% FI$, where `b` is a column vector of variable coefficient estimates and $FI$ is an estimate of the corresponding Fisher information matrix.

The auxiliary functions `lmHmat`, `ldaHmat`, `glhHmat` and `glmHmat` are provided to automatically create the matrices `mat` and `H` in all the cases considered.

**Value**

A list with five items:

- **subsets**
  An $n_{sol} \times k_{max} \times \text{length}(\text{kmin}:\text{kmax})$ 3-dimensional array, giving for each cardinality (dimension 3) and each solution (dimension 1) the list of variables (referenced by their row/column numbers in matrix `mat`) in the subset (dimension 2). (For cardinalities smaller than $k_{max}$, the extra final positions are set to zero).

- **values**
  An $n_{sol} \times \text{length}(\text{kmin}:\text{kmax})$ matrix, giving for each cardinality (columns), the criterion values of the $n_{sol}$ (rows) solutions obtained.

- **bestvalues**
  A length($\text{kmin}:\text{kmax}$) vector giving the best values of the criterion obtained for each cardinality.

- **bestsets**
  A length($\text{kmin}:\text{kmax}$) $\times k_{max}$ matrix, giving, for each cardinality (rows), the variables (referenced by their row/column numbers in matrix `mat`) in the best $k$-subset that was found.

- **call**
  The function call which generated the output.

**References**


See Also

rm.coef, rv.coef, gcd.coef, tau2.coef, xi2.coef, zeta2.coef, ccr12.coef, genetic, anneal, eleaps, trim.matrix, lmHmat, ldaHmat, glhHmat, glmHmat.

Examples

### 1) For illustration of use, a small data set with very few iterations of the algorithm.
Subsets of 2 and of 3 variables are sought using the RM criterion.

```r
data(swiss)
improve(cor(swiss),2,3,nsol=4,criterion="GCD")
```

```r
## $subsets
## , , Card.2
##   Var.1 Var.2 Var.3
## Solution 1  3  6  0
## Solution 2  3  6  0
## Solution 3  3  6  0
## Solution 4  3  6  0
##
## , , Card.3
##   Var.1 Var.2 Var.3
## Solution 1  4  5  6
## Solution 2  4  5  6
## Solution 3  4  5  6
## Solution 4  4  5  6

## $values
##   card.2 card.3
## Solution 1 0.8487026 0.925372
## Solution 2 0.8487026 0.925372
## Solution 3 0.8487026 0.925372
## Solution 4 0.8487026 0.925372

## $bestvalues
##      Card.2 Card.3
## 0.8487026 0.925372

## $bestsets
##   Var.1 Var.2 Var.3
## Card.2  3  6  0
## Card.3  4  5  6

## $call
# improve(cor(swiss), 2, 3, nsol = 4, criterion = "GCD")

#  2) Forcing the inclusion of variable 1 in the subset

improve(cor(swiss), 2, 3, nsol = 4, criterion = "GCD", include = c(1))

# $subsets
#
#
## Card. 2
##
## | Var.1 | Var.2 | Var.3 |
##|-------|-------|-------|
##| 1     | 6     | 0     |
##| 1     | 6     | 0     |
##| 1     | 6     | 0     |
##| 1     | 6     | 0     |
##
## Card. 3
##
## | Var.1 | Var.2 | Var.3 |
##|-------|-------|-------|
##| 1     | 5     | 6     |
##| 1     | 5     | 6     |
##| 1     | 5     | 6     |
##| 1     | 5     | 6     |

# $values

## card. 2  card. 3
## Solution 1 0.7284477 0.8048528
## Solution 2 0.7284477 0.8048528
## Solution 3 0.7284477 0.8048528
## Solution 4 0.7284477 0.8048528

# $bestvalues

## Card. 2 Card. 3
## 0.7284477 0.8048528

# $bestsets

## Card. 2 Card. 3
## 1  6  0
## 1  5  6

# $call

#improve(cor(swiss), 2, 3, nsol = 4, criterion = "GCD", include = c(1))

#  3) An example of subset selection in the context of Multiple Linear Regression. Variable 5 (average car price) in the Cars93 MASS library data set is regressed on 13 other variables. Three variable subsets of
## cardinalities 4, 5 and 6 are requested, using the "XI_2" criterion which,
in the case of a Linear Regression, is merely the standard Coefficient of
Determination, $R^2$ (as are the other three criteria for the
multivariate linear hypothesis, "TAU_2", "CCR1_2" and "ZETA_2").

library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,5])

names(Cars93[,5,drop=FALSE])
## [1] "Price"

colnames(CarsHmat$mat)
## [1] "MPG.city" "MPG.highway" "EngineSize"
## [4] "Horsepower" "RPM" "Rev.per.mile"
## [7] "Fuel.tank.capacity" "Passengers" "Length"
## [10] "Wheelbase" "Width" "Turn.circle"
## [13] "Weight"

improve(CarsHmat$mat, kmin=4, kmax=6, H=CarsHmat$H, r=1, crit="xi2", nsol=3)

## $subsets
## , , Card.4
##
##     Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1  3  4  11  13  0  0
## Solution 2  3  4  11  13  0  0
## Solution 3  4  5  10  11  0  0
##
## , , Card.5
##
##     Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1  3  4  8  11  13  0
## Solution 2  4  5 10  11  12  0
## Solution 3  4  5  10  11  12  0
##
## , , Card.6
##
##     Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1  4  5  6  10  11  12
## Solution 2  4  5  8  10  11  12
## Solution 3  4  5  9  10  11  12
##
## $values
## card.4 card.5 card.6
## Solution 1 0.6880773 0.6899182 0.7270257
## Solution 2 0.6880773 0.7241457 0.7271056
## Solution 3 0.7143794 0.7241457 0.7310150
##
## $bestvalues
## Card.4 Card.5 Card.6
## 0.7143794 0.7241457 0.7310150

## $bestsets
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Card.4 4 5 10 11 0 0
## Card.5 4 5 10 11 12 0
## Card.6 4 5 9 10 11 12

## $call
## improve(mat = CarsHmat$mat, kmin = 4, kmax = 6, nsol = 3, criterion = "xi2",
## H = CarsHmat$H, r = 1)

## 4) A Linear Discriminant Analysis example with a very small data set.
## We consider the Iris data and three groups, defined by species (setosa, versicolor and virginica). The goal is to select the 2- and 3-variable subsets that are optimal for the linear discrimination (as measured by the "TAU_2" criterion).

data(iris)
irisHmat <- ldaHmat(iris[,1:4],iris$Species)
improve(irisHmat$mat,kmin=2,kmax=3,H=irisHmat$H,r=2,crit="ccr12")

## $subsets
## , , Card.2
## #
## # Var.1 Var.2 Var.3
## # Solution 1 2 3 0
## # , , Card.3
## #
## # Var.1 Var.2 Var.3
## # Solution 1 2 3 4

## $values
## card.2 card.3
## Solution 1 0.8079476 0.8419635

## $bestvalues
## Card.2 Card.3
## 0.8079476 0.8419635

## $bestsets
## Var.1 Var.2 Var.3
## Card.2 2 3 0
## Card.3 2 3 4

## $call
## improve(mat = irisHmat$mat, kmin = 2, kmax = 3, criterion = "tau2", H = irisHmat$H, r = 2)
## --------------------------------------------------------------------

## 5) An example of subset selection in the context of a Canonical Correlation Analysis. Two groups of variables within the Cars93 MASS library data set are compared. The goal is to select 4- to 6-variable subsets of the 13-variable 'X' group that are optimal in terms of preserving the canonical correlations, according to the "ZETA_2" criterion (Warning: the 3-variable 'Y' group is kept intact; subset selection is carried out in the 'X' group only). The 'tolsym' parameter is used to relax the symmetry requirements on the effect matrix H which, for numerical reasons, is slightly asymmetric. Since corresponding off-diagonal entries of matrix H are different, but by less than tolsym, H is replaced by its symmetric part: (H+t(H))/2.

library(MASS)
data(Cars93)
CarsHmat <- lmHmat(Cars93[,c(7:8,12:15,17:22,25)],Cars93[,4:6])
names(Cars93[,4:6])
colnames(CarsHmat$mat)
## [1] "MPG.city" "MPG.highway" "EngineSize"
## [4] "Horsepower" "RPM" "Rev.per.mile"
## [7] "Fuel.tank.capacity" "Passengers" "Length"
## [10] "Wheelbase" "Width" "Turn.circle"
## [13] "Weight"

improve(CarsHmat$mat, kmin=4, kmax=6, H=CarsHmat$H, r=3, crit="zeta2", tolsym=1e-9)

## $subsets
## , , Card.4
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 3 4 11 13 0 0
## , , Card.5
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 3 4 9 11 13 0
## , , Card.6
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Solution 1 3 4 5 9 10 11
## $values
## card.4  card.5  card.6
## Solution 1 0.4626035 0.4875495 0.5071096
##
## $bestvalues
## Card.4  Card.5  Card.6
## 0.4626035 0.4875495 0.5071096
##
## $bestsets
## Var.1 Var.2 Var.3 Var.4 Var.5 Var.6
## Card.4 3 4 11 13 0 0
## Card.5 3 4 9 11 13 0
## Card.6 3 4 5 9 10 11
##
## $call
## improve(mat = CarsHmat$mat, kmin = 4, kmax = 6, criterion = "zeta2",
## H = CarsHmat$H, r = 3, tolsym = 1e-09)
##
## Warning message:
## The effect description matrix (H) supplied was slightly asymmetric:
## symmetric entries differed by up to 3.63797880709171e-12.
## (less than the 'tolsym' parameter).
## The H matrix has been replaced by its symmetric part.
## in: validnovcrit(mat, criterion, H, r, p, tolval, tolsym)

6) An example of variable selection in the context of a logistic regression model. We consider the last 100 observations of the iris data set (versicolor and virginica species) and try to find the best variable subsets for the model that takes species as response variable.

data(iris)
iris2sp <- iris[iris$Species != "setosa",]
logrfit <- glm(Species ~ Sepal.Length + Sepal.Width + Petal.Length + Petal.Width, iris2sp,family=binomial)
Hmat <- glmHmat(logrfit)
improve(Hmat$mat,1,3,H=Hmat$H,r=1,criterion="Wald")

## $subsets
## , , Card.1
#### Var.1 Var.2 Var.3
## Solution 1 4 0 0
##
## , , Card.2
#### Var.1 Var.2 Var.3
## Solution 1 1 3 0
ldaHmat

## , , Card.3
## Var.1 Var.2 Var.3
## Solution 1 2 3 4

## $values
## card.1 card.2 card.3
## Solution 1 4.894554 3.522885 1.060121

## $bestvalues
## Card.1 Card.2 Card.3
## 4.894554 3.522885 1.060121

## $bestsets
## Var.1 Var.2 Var.3
## Card.1 4 0 0
## Card.2 1 3 0
## Card.3 2 3 4

## $call
## improve(mat = Hmat$mat, kmin = 1, kmax = 3, criterion = "Wald",
## H = Hmat$H, r = 1)

# It should be stressed that, unlike other criteria in the subselect package, the Wald criterion is not bounded above by 1 and is a decreasing function of subset quality, so that the 3-variable subsets do, in fact, perform better than their smaller-sized counterparts.

---

**ldaHmat**

*Total and Between-Group Deviation Matrices in Linear Discriminant Analysis*

**Description**

Computes total and between-group matrices of Sums of Squares and Cross-Product (SSCP) deviations in linear discriminant analysis. These matrices may be used as input to the variable selection search routines `anneal`, `genetic improve`, or `eleaps`.

**Usage**

```r
## Default S3 method:
daHmat(x, grouping, ...)
## S3 method for class 'data.frame'
```
```r
ldaHmat(x, grouping, ...)
## S3 method for class 'formula'
ldaHmat(formula, data = NULL, ...)
```

### Arguments

- **x**: A matrix or data frame containing the discriminators for which the SSCP matrix is to be computed.
- **grouping**: A factor specifying the class for each observation.
- **formula**: A formula of the form `groups ~ x1 + x2 + ...` That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
- **data**: Data frame from which variables specified in `formula` are preferentially to be taken.
- **...**: Further arguments for the method.

### Value

A list with four items:

- **mat**: The total SSCP matrix
- **H**: The between-groups SSCP matrix
- **r**: The expected rank of the H matrix which equals the minimum between the number of discriminators and the number of groups minus one. The true rank of H can be different from r if the discriminators are linearly dependent.
- **call**: The function call which generated the output.

### See Also

`anneal`, `genetic`, `improve`, `eleaps`, `lda`.

### Examples

```r
##--------------------------------------------------------------------
## An example with a very small data set. We consider the Iris data
## and three groups, defined by species (setosa, versicolor and
## virginica).

data(iris)
irisHmat <- ldaHmat(iris[1:4], iris$Species)
irisHmat

##$mat
##             Sepal.Length  Sepal.Width Petal.Length Petal.Width
##Sepal.Length 102.168333  -6.322667    189.8730    76.92433
##Sepal.Width  -6.322667    28.306933   -49.1188   -18.12427
##Petal.Length 189.873000   -49.118800   464.3254   193.04580
```
Description

Computes total and effect matrices of Sums of Squares and Cross-Product (SSCP) deviations, divided by a normalizing constant, in linear regression or canonical correlation analysis. These matrices may be used as input to the variable selection search routines `anneal`, `genetic improve` or `eleaps`.

Usage

```r
## Default S3 method:
lmHmat(x,y,...)

## S3 method for class 'data.frame'
lmHmat(x,y,...)

## S3 method for class 'formula'
lmHmat(formula,data=NULL,...)

## S3 method for class 'lm'
lmHmat(fitdlmmodel,...)
```

Arguments

- `x`: A matrix or data frame containing the variables for which the SSCP matrix is to be computed.
lmHmat

**y**
A matrix or data frame containing the set of fixed variables, the association of x is to be measured with.

**formula**
A formula of the form 'y ~ x1 + x2 + ...'. That is, the response is the set of fixed variables and the right hand side specifies the variables whose subsets are to be compared.

**data**
Data frame from which variables specified in 'formula' are preferentially to be taken.

**fitdlmmodel**
An object of class lm, as produced by R’s lm function.

**...**
further arguments for the method.

**Details**
Let x and y be two different groups of linearly independent variables observed on the same set of data units. It is well known that the association between x and y can be measured by their squared canonical correlations which may be found as the positive eigenvalues of certain matrix products. In particular, if $T_x$ and $H_{x/y}$ denote SSCP matrices of deviations from the mean, respectively for the original x variables ($T_x$) and for their orthogonal projections onto the space spanned by the y’s ($H_{x/y}$), then the positive eigenvalues of $T_x^{-1}H_{x/y}$ equal the squared correlations between x and y. Alternatively these correlations could also be found from $T_y^{-1}H_{y/x}$ but here, assuming a goal of comparing x’s subsets for a given fixed set of y’s, we will focus on the former product. lmHmat computes a scaled version of $T_x$ and $H_{x/y}$ such that $T_x$ is converted into a covariance matrix. These matrices can be used as input to the search routines anneal, genetic, improve and eleaps that try to select x subsets based on several functions of their squared correlations with y. We note that when there is only one variable in the y set, this is equivalent to selecting predictors for linear regression based on the traditional coefficient of determination.

**Value**
A list with four items:

- **mat**  The total SSCP matrix divided by nrow(x)-1
- **H**  The effect SSCP matrix divided by nrow(x)-1
- **r**  The expected rank of the H matrix which, under the assumption of linear independence, equals the minimum between the number of variables in the x and y sets. The true rank of H can be different from r if the linear independence condition fails.
- **call**  The function call which generated the output.

**See Also**
anneal, genetic, improve, eleaps, lm.

**Examples**
```r
#------------------

## 1) An example of subset selection in the context of Multiple Linear Regression. Variable 5 (average price) in the Cars93 MASS
```
library is to be regressed on 13 other variables. The goal is to compare subsets of these 13 variables according to their ability to predict car prices.

library(MASS)
data(Cars93)
CarsHmat1 <- lmHmat(Cars93[c(7:8,12:15,17:22,25)],Cars93[5])
CarsHmat1

# $mat
# #MPG.city 31.582281 28.283427 -4.1391655 -1.979799e+02
# #MPG.highway 28.283427 28.427302 -3.4676700 -1.728655e+02
# #EngineSize -4.139165 -3.467670 1.0761220 3.977700e+01
# #Horsepower -197.979897 -172.865475 39.7769986 2.743079e+03
# #RPM 1217.478962 997.335203 -339.1637447 1.146634e+03
# #Rev.per.mile 1941.631019 1555.243104 -424.4118163 -1.561070e+04
# #Fuel.tank.capacity -14.985799 -13.743654 2.5830820 1.225362e+02
# #Passengers -2.433964 -2.583567 0.4017181 5.040907e-01
# #Length -54.673329 -42.267765 11.8197055 4.212964e+02
# #Wheelbase -25.567087 -22.375760 5.1819425 1.738922e+02
# #Width -15.302127 -12.902291 3.3992286 1.275374e+02
# #Turn.circle -12.871061 -10.202782 2.6029453 9.474252e+01
# #Weight -2795.094670 -2549.654628 517.1327139 2.282550e+04
# RPM Rev.per.mile Fuel.tank.capacity Passengers
# #MPG.city 1217.4790 1941.6310 -14.985799 -2.4339645
# #MPG.highway 997.3352 1555.2431 -13.743654 -2.5835671
# #EngineSize -339.1637 -424.4118 2.583082 0.4017181
# #Horsepower 1146.6339 -15610.7497 122.253612 0.5040907
# #RPM 356088.7097 146589.3233 -652.324684 -289.6213184
# #Rev.per.mile 146589.3233 246518.7295 -992.747020 -172.8003740
# #Fuel.tank.capacity -652.3247 -992.7470 10.754271 1.6085203
# #Passengers -289.6213 -172.8004 1.608520 1.0794764
# #Length -3844.9158 -5004.3139 33.063850 7.3626605
# #Wheelbase -1903.7693 -2156.2932 16.944811 4.9177186
# #Width -1217.8933 -1464.3712 9.898282 1.9237962
# #Turn.circle -972.5806 -1173.3281 7.096283 1.5037401
# #Weight -150636.1325 -215349.6757 1729.468468 339.0953717
# Length Wheelbase Width Turn.circle
# #MPG.city -54.67333 -25.567087 -15.302127 -12.071061
# #MPG.highway -42.26777 -22.375760 -12.902291 -10.202782
# #EngineSize 11.81971 5.181942 3.399229 2.602945
# #Horsepower 2.412964 173.892824 127.543712 94.745250
# #RPM -3844.9158 1903.769285 -1217.893268 -972.580645
# #Rev.per.mile -5004.3139 -2156.2932 -1464.3712 -1173.3287
# #Fuel.tank.capacity 33.06385 16.944811 9.898282 7.096283
# #Passengers 7.36267 4.917719 1.923796 1.503740
# #Length 213.22955 82.821973 45.367929 34.780622
# #Wheelbase 82.821974 46.507948 20.803062 15.89936
# #Width 45.36793 20.803062 14.288739 9.962015
# #Turn.circle 34.78062 15.89936 9.962015 10.389434
# #Weight 6945.16129 3507.549088 1950.471599 1479.365358
# Weight
##MPG.city -2795.8947
##MPG.highway -2549.6546
##EngineSize 517.1327
##Horsepower 22825.5049
##RPM -150636.1325
##Rev.per.mile -215349.6757
##Fuel.tank.capacity 1729.4683
##Passengers 339.0954
##Length 6945.1613
##Wheelbase 3507.5491
##Width 1950.4716
##Turn.circle 1479.3654
##Weight 347977.8927

###$H$

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## Length Wheelbase Width Turn.circle

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###lmHmat
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## Width  12.673619  5.8864067  2.9698426  2.18072961
## Turn.circle  9.306128  4.3223372  2.1807296  1.60129079
## Weight  2807.593227  1304.018621  657.910722  483.09812289
##
## Weight
##
## MPG.city  -1275.61396
## MPG.highway  -1141.25690
## EngineSize  236.59997
## Horsepower  15760.33711
## RPM  -1128.79998
## Rev.per.mile  -80823.45772
## Fuel.tank.capacity  775.56465
## Passengers  22.95016
## Length  2807.59323
## Wheelbase  1304.01862
## Width  657.91072
## Turn.circle  483.09812
## Weight  145747.29199

## $r
## [1] 1

## $call
## lmHmat.default.frame(x = Cars93[,7:8,12:15,17:22,25], y = Cars93[,5])

## 2) An example of subset selection in the context of Canonical Correlation Analysis. Two groups of variables within the Cars93 MASS library data set are compared. The first group (variables 4th, 5th and 6th) relates to price, while the second group is formed by 13 variables that describe several technical car specifications. The goal is to select subsets of the second group that are optimal in terms of preserving the canonical correlations with the variables in the first group (Warning: the 3-variable "response" group is kept intact; subset selection is to be performed only in the 13-variable group).

library(MASS)
data(Cars93)
CarsHmat2 <- lmHmat(Cars93[,7:8,12:15,17:22,25],Cars93[,4:6])
names(Cars93[,4:6])

CarsHmat2

## $mat
##
## Mint.Price Price Max.Price
## Mint.Price  1.00000  0.99999  0.99999
## Price     0.99999  1.00000  0.99999
## Max.Price  0.99999  0.99999  1.00000

library(MASS)
data(Cars93)
CarsHmat2 <- lmHmat(Cars93[,7:8,12:15,17:22,25],Cars93[,4:6])
names(Cars93[,4:6])

CarsHmat2

## $mat
##
## Mint.Price Price Max.Price
## Mint.Price  1.00000  0.99999  0.99999
## Price     0.99999  1.00000  0.99999
## Max.Price  0.99999  0.99999  1.00000

library(MASS)
data(Cars93)
CarsHmat2 <- lmHmat(Cars93[,7:8,12:15,17:22,25],Cars93[,4:6])
names(Cars93[,4:6])

CarsHmat2

## $mat
##
## Mint.Price Price Max.Price
## Mint.Price  1.00000  0.99999  0.99999
## Price     0.99999  1.00000  0.99999
## Max.Price  0.99999  0.99999  1.00000

library(MASS)
data(Cars93)
CarsHmat2 <- lmHmat(Cars93[,7:8,12:15,17:22,25],Cars93[,4:6])
names(Cars93[,4:6])

CarsHmat2

## $mat
##
## Mint.Price Price Max.Price
## Mint.Price  1.00000  0.99999  0.99999
## Price     0.99999  1.00000  0.99999
## Max.Price  0.99999  0.99999  1.00000

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CarsHmat2 <- lmHmat(Cars93[,7:8,12:15,17:22,25],Cars93[,4:6])
names(Cars93[,4:6])

CarsHmat2

## $mat
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## Mint.Price Price Max.Price
## Mint.Price  1.00000  0.99999  0.99999
## Price     0.99999  1.00000  0.99999
## Max.Price  0.99999  0.99999  1.00000

library(MASS)
data(Cars93)
CarsHmat2 <- lmHmat(Cars93[,7:8,12:15,17:22,25],Cars93[,4:6])
names(Cars93[,4:6])

CarsHmat2

## $mat
##
## Mint.Price Price Max.Price
## Mint.Price  1.00000  0.99999  0.99999
## Price     0.99999  1.00000  0.99999
## Max.Price  0.99999  0.99999  1.00000
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Computes the RM coefficient for variable subset selection

Description
Computes the RM coefficient, measuring the similarity of the spectral decompositions of a \( p \)-variable data matrix, and of the matrix which results from regressing all the variables on a subset of only \( k \) variables.

Usage
\[ \text{rm.coef(mat, indices)} \]

Arguments
- `mat`: the full data set’s covariance (or correlation) matrix
- `indices`: a numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different \( k \)-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.

Details
Computes the RM coefficient that measures the similarity of the spectral decompositions of a \( p \)-variable data matrix, and of the matrix which results from regressing those variables on a subset (given by "indices") of the variables. Input data is expected in the form of a (co)variance or correlation matrix. If a non-square matrix is given, it is assumed to be a data matrix, and its correlation matrix is used as input.

The definition of the RM coefficient is as follows:

\[
RM = \sqrt{\frac{\text{tr}(X^tP_vX)}{X^tX}}
\]

where \( X \) is the full (column-centered) data matrix and \( P_v \) is the matrix of orthogonal projections on the subspace spanned by a \( k \)-variable subset.
This definition is equivalent to:

\[ RM = \sqrt{\frac{\sum_{i=1}^{p} \lambda_i(r)^2}{\sum_{j=1}^{p} \lambda_j}} \]

where \( \lambda_i \) stands for the \( i \)-th largest eigenvalue of the covariance matrix defined by \( X \) and \( r \) stands for the multiple correlation between the \( i \)-th Principal Component and the \( k \)-variable subset.

These definitions are also equivalent to the expression used in the code, which only requires the covariance (or correlation) matrix of the data under consideration.

The fact that indices can be a matrix or 3-d array allows for the computation of the RM values of subsets produced by the search functions `anneal`, `genetic` and `improve` (whose output option `$subsets` are matrices or 3-d arrays), using a different criterion (see the example below).

**Value**

The value of the RM coefficient.

**References**


**Examples**

```r
## An example with a very small data set.

data(iris3)
x<-iris3[,1]
rm.coef(var(x),c(1,3))
## [1] 0.8724422

## An example computing the RMs of three subsets produced when the
## anneal function attempted to optimize the RV criterion (using an
## absurdly small number of iterations).

data(swiss)
rvresults<-anneal(cor(swiss),2,nsol=4,niter=5,criterion="Rv")
rm.coef(cor(swiss),rvresults$subsets)
## Card.2
##Solution 1 0.7982296
##Solution 2 0.7945390
##Solution 3 0.7649296
##Solution 4 0.7623326
```
rv.coef

Computes the RV-coefficient applied to the variable subset selection problem

Description

Computes the RV coefficient, measuring the similarity (after rotations, translations and global re-sizing) of two configurations of n points given by: (i) observations on each of p variables, and (ii) the regression of those p observed variables on a subset of the variables.

Usage

rv.coef(mat, indices)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>mat</td>
<td>the full data set’s covariance (or correlation) matrix</td>
</tr>
<tr>
<td>indices</td>
<td>a numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different k-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.</td>
</tr>
</tbody>
</table>

Details

Input data is expected in the form of a (co)variance or correlation matrix of the full data set. If a non-square matrix is given, it is assumed to be a data matrix, and its correlation matrix is used as input. The subset of variables on which the full data set will be regressed is given by indices.

The RV-coefficient, for a (column-centered) data matrix (with p variables/columns) X, and for the regression of these columns on a k-variable subset, is given by:

$$RV = \frac{\text{tr}(XX^t \cdot (P_vX)(P_vX)^t)}{\sqrt{\text{tr}((XX^t)^2) \cdot \text{tr}(((P_vX)(P_vX)^t)^2)}}$$

where $P_v$ is the matrix of orthogonal projections on the subspace defined by the k-variable subset.

This definition is equivalent to the expression used in the code, which only requires the covariance (or correlation) matrix of the data under consideration.

The fact that indices can be a matrix or 3-d array allows for the computation of the RV values of subsets produced by the search functions anneal, genetic and improve (whose output option $subsets$ are matrices or 3-d arrays), using a different criterion (see the example below).

Value

The value of the RV-coefficient.

References

Examples

# A simple example with a trivially small data set

data(iris3)
x <- iris3[,1]
rvec <- rvec(x, c(1,3))
## [1] 0.8659685

## An example computing the RVs of three subsets produced when the
## anneal function attempted to optimize the RM criterion (using an
## absurdly small number of iterations).

data(swiss)
rmresults <- anneal(cor(swiss), 2, nsol=4, niter=5, criterion="Rm")
rv.coef(cor(swiss), rmresults$subsets)
## Card.2
## Solution 1 0.8389669
## Solution 2 0.8663006
## Solution 3 0.8093862
## Solution 4 0.7529066

---

**tau2.coef**

*Computes the Tau squared coefficient for a multivariate linear hypothesis*

---

**Description**

Computes the Tau squared index of "effect magnitude". The maximization of this criterion is equivalent to the minimization of Wilk's lambda statistic.

**Usage**

```r
tau2.coef(mat, H, r, indices, 
tolval=10*.Machine$double.eps, tolsym=1000*.Machine$double.eps)
```

**Arguments**

- **mat**: the Variance or Total sums of squares and products matrix for the full data set.
- **H**: the Effect description sums of squares and products matrix (defined in the same way as the mat matrix).
- **r**: the Expected rank of the H matrix. See the Details below.
- **indices**: a numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different k-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.
tau2.coef

**tolval**

the tolerance level to be used in checks for ill-conditioning and positive-definiteness of the 'total' and 'effects' (H) matrices. Values smaller than *tolval* are considered equivalent to zero.

**tolsym**

the tolerance level for symmetry of the covariance/correlation/total matrix and for the effects (H) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes \((A + t(A))/2\).

**Details**

Different kinds of statistical methodologies are considered within the framework, of a multivariate linear model:

\[ X = A\Psi + U \]

where \(X\) is the (nxp) data matrix of original variables, \(A\) is a known (nxp) design matrix, \(\Psi\) an (qxp) matrix of unknown parameters and \(U\) an (nxp) matrix of residual vectors. The \(\tau^2\) index is related to the traditional test statistic (Wilk’s lambda statistic) and measures the contribution of each subset to an Effect characterized by the violation of a linear hypothesis of the form \(C\Psi = 0\), where \(C\) is a known coefficient matrix of rank \(r\). The Wilk’s lambda statistic \((\Lambda)\) is given by:

\[ \Lambda = \frac{\det(E)}{\det(T)} \]

where \(E\) is the Error matrix and \(T\) is the Total matrix. The index \(\tau^2\) is related to the Wilk’s lambda statistic \((\Lambda)\) by:

\[ \tau^2 = 1 - \Lambda^{(1/r)} \]

where \(r\) is the rank of \(H\) the Effect matrix.

The fact that indices can be a matrix or 3-d array allows for the computation of the \(\tau^2\) values of subsets produced by the search functions `anneal`, `genetic`, `improve` and `eleaps` (whose output option `$subsets` are matrices or 3-d arrays), using a different criterion (see the example below).

**Value**

The value of the \(\tau^2\) coefficient.

**Examples**

```r
## -----------------------------------------------
## 1) A Linear Discriminant Analysis example with a very small data set.
## We considered the Iris data and three groups,
## defined by species (setosa, versicolor and virginica).

data(iris)
irisHmat <- ldaHmat(iris[1:4],iris$Species)
tau2.coef(irisHmat$mat,H=irisHmat$H,r=2,c(1,3))
## [1] 0.8003044
```
## 2) An example computing the value of the tau_2 criterion for two subsets produced when the anneal function attempted to optimize the xi_2 criterion (using an absurdly small number of iterations).

```r
xresults <- anneal(irisHmat$mat, 2, nsol=2, niter=2, criterion="xi2", H=irisHmat$H, r=2)
tau2.coef(irisHmat$mat, H=irisHmat$H, r=2, xresults$subsets)
```

```
Card.2
Solution 1 0.8079476
Solution 2 0.7907710
```

---

**trim.matrix**

*Given an ill-conditioned square matrix, deletes rows/columns until a well-conditioned submatrix is obtained.*

### Description

This function seeks to deal with ill-conditioned matrices, for which the search algorithms of optimal k-variable subsets could encounter numerical problems. Given a square matrix `mat` which is assumed positive semi-definite, the function checks whether it has reciprocal of the 2-norm condition number (i.e., the ratio of the smallest to the largest eigenvalue) smaller than `tolval`. If not, the matrix is considered well-conditioned and remains unchanged. If the ratio of the smallest to largest eigenvalue is smaller than `tolval`, an iterative process is begun, which deletes rows/columns (using Jolliffe's method for subset selections described on pg. 138 of the Reference below) until a principal submatrix with reciprocal of the condition number larger than `tolval` is obtained.

### Usage

`trim.matrix(mat, tolval=10*.Machine$double.eps)`

### Arguments

- **mat**: a symmetric matrix, assumed positive semi-definite.
- **tolval**: the tolerance value for the reciprocal condition number of matrix `mat`.

### Details

For the given matrix `mat`, eigenvalues are computed. If the ratio of the smallest to the largest eigenvalue is less than `tolval`, matrix `mat` remains unchanged and the function stops. Otherwise, an iterative process is begun, in which the eigenvector associated with the smallest eigenvalue is considered and its largest (in absolute value) element is identified. The corresponding row/column are deleted from matrix `mat` and the eigendecomposition of the resulting submatrix is computed.
This iterative process stops when the ratio of the smallest to largest eigenvalue is not smaller than \( \text{tolval} \).

The function checks whether the input matrix is square, but not whether it is positive semi-definite. This \texttt{trim.matrix} function can be used to delete rows/columns of square matrices, until only non-negative eigenvalues appear.

\textbf{Value}

Output is a list with four items:

- \textit{trimmedmat} is a principal submatrix of the original matrix, with the ratio of its smallest to largest eigenvalues no smaller than \( \text{tolval} \). This matrix can be used as input for the search algorithms in this package.
- \textit{numbers.dropped} is a list of the integer numbers of the original variables that were discarded.
- \textit{names.dropped} is a list of the original column numbers of the variables that were discarded.
- \textit{size} is the size of the output matrix.

\textbf{Note}

When the \texttt{trim.matrix} function is used to produce a well-conditioned matrix for use with the \texttt{anneal}, \texttt{genetic}, \texttt{improve} or \texttt{eleaps} functions, care must be taken in interpreting the output of those functions. In those search functions, the selected variable subsets are specified by variable numbers, and those variable numbers indicate the position of the variables in the input matrix. Hence, if a trimmed matrix is supplied to functions \texttt{anneal}, \texttt{genetic}, \texttt{improve} or \texttt{eleaps}, variable numbers refer to the \textit{trimmed matrix}.

\textbf{References}


\textbf{Examples}

```
# a trivial example, for illustration of use: creating an extra column,
# as the sum of columns in the "iris" data, and then using the function
# \texttt{trim.matrix} to exclude it from the data's correlation matrix

data(iris)
lindepir<-cbind(apply(iris[,-5],1,sum),iris[,-5])
colnames(lindepir)[1]<-"Sum"
cor(lindepir)

###          Sum  Sepal.Length  Sepal.Width Petal.Length Petal.Width
### Sum 1.0000000 0.9409143 -0.2230928 0.9713793 0.9538850
### Sepal.Length 0.9409143 1.0000000 -0.1175698 0.8717538 0.8179411
### Sepal.Width -0.2230928 -0.1175698 1.0000000 -0.4284401 -0.3661259
### Petal.Length 0.9713793 0.8717538 -0.4284401 1.0000000 0.9628654
### Petal.Width  0.9538850 0.8179411 -0.3661259 0.9628654 1.0000000
```
trim.matrix(cor(lindepir))

##$trimmedmat
## Sepal.Length Sepal.Width Petal.Length Petal.Width
## Sepal.Length 1.0000000 -0.1175698 0.8717538 0.8179411
## Sepal.Width -0.1175698 1.0000000 -0.4284401 -0.3661259
## Petal.Length 0.8717538 -0.4284401 1.0000000 0.9628654
## Petal.Width 0.8179411 -0.3661259 0.9628654 1.0000000
##
####$numbers.discarded
## [1] 1
##
####$names.discarded
## [1] "Sum"
##
####$size
## [1] 4

data(swiss)
lindepsw<-cbind(apply(swiss,1,sum),swiss)
colnames(lindepsw)[1]<-"Sum"
trim.matrix(cor(lindepsw))

##$lowrankmat
## Fertility Agriculture examination Education Catholic
## Fertility 1.0000000 0.35307918 -0.6458827 -0.66378886 0.4636847
## Agriculture 0.3530792 1.00000000 -0.6865422 -0.63952252 0.4010951
## Examination -0.6458827 -0.68654221 1.0000000 0.69841530 -0.5727418
## Education -0.6637889 -0.63952252 0.6984153 1.00000000 -0.1538589
## Catholic 0.4636847 0.40109505 -0.5727418 -0.15385892 1.0000000
## Infant.Mortality 0.4165560 -0.06085861 -0.11402160 -0.09932185 0.1754959
##
####$numbers.discarded
## [1] 1
##
####$names.discarded
## [1] "Sum"
##
####$size
## [1] 6
wald.coef

Wald statistic for variable selection in generalized linear models

Description

Computes the value of Wald’s statistic, testing the significance of the excluded variables, in the context of variable subset selection in generalized linear models.

Usage

wald.coef(mat, H, indices,
tolval=10*.Machine$double.eps, tolsym=1000*.Machine$double.eps)

Arguments

mat
An estimate (Fi) of Fisher’s information matrix for the full model variable-coefficient estimates.

H
A matrix product of the form Fi ★ b ★ t(b) ★ Fi where b is a vector of variable-coefficient estimates.

indices
A numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different k-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.

tolval
The tolerance level to be used in checks for ill-conditioning and positive-definiteness of the Fisher Information and the auxiliary (H) matrices. Values smaller than tolval are considered equivalent to zero.

tolsym
The tolerance level for symmetry of the Fisher Information and the auxiliary (H) matrices. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes (A+t(A))/2.

Details

Variable selection in the context of generalized linear models is typically based on the minimization of statistics that test the significance of excluded variables. In particular, the likelihood ratio, Wald’s, Rao’s and some adaptations of such statistics, are often proposed as comparison criteria for variable subsets of the same dimensionality. All these statistics are asymptotically equivalent and can be converted into information criteria, like the AIC, that are also able to compare subsets of different dimensionalities (see references [1] and [2] for further details).

Among these criteria, Wald’s statistic has some computational advantages because it can always be derived from the same (concerning the full model) maximum likelihood and Fisher information estimates. In particular, if \( W_{all} \) is the value of the Wald statistic testing the significance of the full covariate vector, b and Fi are coefficient and Fisher information estimates and H is an auxiliary rank-one matrix given by \( H = FI \%*% b \%*% t(b) \%*% FI \), it follows that the value of Wald’s statistic for the excluded variables (\( W_{exec} \)) in a given subset is given by

\[
W_{exec} = W_{all} - tr(FI_{indices}^{-1}H_{indices}),
\]
where $F_{indices}$ and $H_{indices}$ are the portions of the FI and H matrices associated with the selected variables.

The FI and H matrices can be retrieved (from a glm object) by the `glmHmat` function and may be used as input to the search functions `anneal`, `genetic`, `improve` and `eleaps`. The Wald function computes the value of Wald statistic from these matrices for a subset specified by indices.

The fact that indices can be a matrix or 3-d array allows for the computation of the Wald statistic values of subsets produced by the search functions `anneal`, `genetic`, `improve` and `eleaps` (whose output option `$subsets` are matrices or 3-d arrays), using a different criterion (see the example below).

**Value**

The value of the Wald statistic.

**References**


**Examples**

```r
## An example of variable selection in the context of binary response
## regression models. The logarithms and original physical measurements
## of the "Leptograpsus variegatus crabs" considered in the MASS crabs
## data set are used to fit a logistic model that takes the sex of each crab
## as the response variable.

library(MASS)
data(crabs)
lFL <- log(crabs$FL)
lRW <- log(crabs$RW)
lCL <- log(crabs$CL)
lCW <- log(crabs$CW)
logrfit <- glm(sex ~ FL + RW + CL + CW + lFL + lRW + lCL + lCW, crabs, family=binomial)

## Warning message:
## fitted probabilities numerically 0 or 1 occurred in: glm.fit(x = X, y = Y,
## weights = weights, start = start, etastart = etastart,

lHmat <- glmHmat(logrfit)
wald.coef(lHmat$mat,lHmat$H,c(1,6,7),tolsym=1E-06)
## [1] 2.286739
```
## The covariance/total matrix supplied was slightly asymmetric:
## symmetric entries differed by up to 6.57252030578093e-14.
## (less than the 'tolsym' parameter).
## It has been replaced by its symmetric part.
## in: validmat(mat, p, tolval, tolsym)

## 2) An example computing the value of the Wald statistic in a logistic
## model for five subsets produced when a probit model was originally
## considered

library(MASS)
data(crabs)
lFL <- log(crabs$FL)
lRW <- log(crabs$RW)
lCL <- log(crabs$CL)
lCW <- log(crabs$CW)
probfit <- glm(sex ~ FL + RW + CL + CW + lFL + lRW + lCL + lCW,
crabs,family=binomial(link=probit))
## Warning message:
## fitted probabilities numerically 0 or 1 occurred in: glm.fit(x = X, y = Y,
## weights = weights, start = start, etastart = etastart)

pHmat <- glmHmat(probfit)
probresults <- eleaps(pHmat$mat,kmin=3,kmax=3,nsol=5,criterion="Wald",H=pHmat$H,
r=1,tolsym=1E-10)
## Warning message:
## The covariance/total matrix supplied was slightly asymmetric:
## symmetric entries differed by up to 3.14059889205964e-12.
## (less than the 'tolsym' parameter).
## It has been replaced by its symmetric part.
## in: validmat(mat, p, tolval, tolsym)

logrfit <- glm(sex ~ FL + RW + CL + CW + lFL + lRW + lCL + lCW,
crabs,family=binomial)
## Warning message:
## fitted probabilities numerically 0 or 1 occurred in: glm.fit(x = X, y = Y,
## weights = weights, start = start, etastart = etastart)

lHmat <- glmHmat(logrfit)
wald.coef(lHmat$mat,H=lHmat$H,probresults$subsets,tolsym=1e-06)
## Card.3
## Solution 1 2.286739
## Solution 2 2.595165
## Solution 3 2.585149
## Solution 4 2.669059
## Solution 5 2.690954
## Warning message:
xi2.coef

## The covariance/total matrix supplied was slightly asymmetric:
## symmetric entries differed by up to 6.57252030578093e-14.
## (less than the 'tolsym' parameter).
## It has been replaced by its symmetric part.
## in: validmat(mat, p, tolval, tolsym)

### xi2.coef

Computes the Xi squared coefficient for a multivariate linear hypothesis

#### Description

Computes the Xi squared index of "effect magnitude". The maximization of this criterion is equivalent to the maximization of the traditional test statistic, the Bartlett-Pillai trace.

#### Usage

```
xi2.coef(mat, H, r, indices,
tolval=10*.Machine$double.eps, tolsym=1000*.Machine$double.eps)
```

#### Arguments

- **mat**
  - the Variance or Total sums of squares and products matrix for the full data set.
- **H**
  - the Effect description sums of squares and products matrix (defined in the same way as the mat matrix).
- **r**
  - the Expected rank of the H matrix. See the Details below.
- **indices**
  - a numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different k-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.
- **tolval**
  - the tolerance level to be used in checks for ill-conditioning and positive-definiteness of the 'total' and 'effects' (H) matrices. Values smaller than tolval are considered equivalent to zero.
- **tolsym**
  - the tolerance level for symmetry of the covariance/correlation/total matrix and for the effects (H) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes (A+t(A))/2.
Details

Different kinds of statistical methodologies are considered within the framework of a multivariate linear model:

\[ X = A \Psi + U \]

where \( X \) is the (nxp) data matrix of original variables, \( A \) is a known (nxp) design matrix, \( \Psi \) an (qxpx) matrix of unknown parameters and \( U \) an (nxp) matrix of residual vectors. The Xi squared index is related to the traditional test statistic (Bartlett-Pillai trace) and measures the contribution of each subset to an Effect characterized by the violation of a linear hypothesis of the form \( C \Psi = 0 \), where \( C \) is a known coefficient matrix of rank \( r \). The Bartlett-Pillai trace \( (P) \) is given by: \( P = tr(HT^{-1}) \) where \( H \) is the Effect matrix and \( T \) is the Total matrix. The Xi squared index is related to Bartlett-Pillai trace \( (P) \) by:

\[ \xi^2 = \frac{P}{r} \]

where \( r \) is the rank of \( H \) matrix.

The fact that indices can be a matrix or 3-d array allows for the computation of the Xi squared values of subsets produced by the search functions \texttt{anneal}, \texttt{genetic}, \texttt{improve} and \texttt{eleaps} (whose output option $subsets$ are matrices or 3-d arrays), using a different criterion (see the example below).

Value

The value of the \( \xi^2 \) coefficient.

Examples

```r
## ---------------------------------------------------------------
## 1) A Linear Discriminant Analysis example with a very small data set.
## We considered the Iris data and three groups, defined by species (setosa, versicolor and virginica).

data(iris)
irisHmat <- ldaHmat(iris[1:4],iris$Species)
xi2.coef(irisHmat$mat,H=irisHmat$H,r=2,c(1,3))
## [1] 0.4942503
## ---------------------------------------------------------------

## 2) An example computing the value of the xi_2 criterion for two subsets produced when the anneal function attempted to optimize the tau_2 criterion (using an absurdly small number of iterations).

tauresults<-anneal(irisHmat$mat,2,nsol=2,niter=2,criterion="tau2",H=irisHmat$H,r=2)
xi2.coef(irisHmat$mat,H=irisHmat$H,r=2,tauresults$subsets)
## Card.2
##Solution 1 0.5718811
##Solution 2 0.5232262
```
## zeta2.coef

*Computes the Zeta squared coefficient for a multivariate linear hypothesis*

### Description

Computes the Zeta squared index of "effect magnitude". The maximization of this criterion is equivalent to the maximization of the traditional test statistic, the Lawley-Hotelling trace.

### Usage

\[
\text{zeta2.coef}(\text{mat}, \text{H}, r, \text{indices}, \text{tolval}=10 \cdot \text{Machine$double.eps}, \text{tolsym}=1000 \cdot \text{Machine$double.eps})
\]

### Arguments

- **mat**: the Variance or Total sums of squares and products matrix for the full data set.
- **H**: the Effect description sums of squares and products matrix (defined in the same way as the mat matrix).
- **r**: the Expected rank of the H matrix. See the Details below.
- **indices**: a numerical vector, matrix or 3-d array of integers giving the indices of the variables in the subset. If a matrix is specified, each row is taken to represent a different k-variable subset. If a 3-d array is given, it is assumed that the third dimension corresponds to different cardinalities.
- **tolval**: the tolerance level to be used in checks for ill-conditioning and positive-definiteness of the 'total' and 'effects' (H) matrices. Values smaller than tolval are considered equivalent to zero.
- **tolsym**: the tolerance level for symmetry of the covariance/correlation/total matrix and for the effects (H) matrix. If corresponding matrix entries differ by more than this value, the input matrices will be considered asymmetric and execution will be aborted. If corresponding entries are different, but by less than this value, the input matrix will be replaced by its symmetric part, i.e., input matrix A becomes \( (A + t(A))/2 \).

### Details

Different kinds of statistical methodologies are considered within the framework, of a multivariate linear model:

\[
X = A\Psi + U
\]

where \( X \) is the (n xp) data matrix of original variables, \( A \) is a known (n xp) design matrix, \( \Psi \) an (q xp) matrix of unknown parameters and \( U \) an (n xp) matrix of residual vectors. The \( \zeta^2 \) index is related to
the traditional test statistic (Lawley-Hotelling trace) and measures the contribution of each subset to an Effect characterized by the violation of a linear hypothesis of the form $C\Psi = 0$, where $C$ is a known coefficient matrix of rank $r$. The Lawley-Hotelling trace is given by: $V = tr(HE^{-1})$ where $H$ is the Effect matrix and $E$ is the Error matrix. The index $\zeta^2$ is related to Lawley-Hotelling trace ($V$) by:

$$\zeta^2 = \frac{V}{V + r}$$

where $r$ is the rank of $H$ matrix.

The fact that indices can be a matrix or 3-d array allows for the computation of the $\zeta^2$ values of subsets produced by the search functions `anneal`, `genetic`, `improve` and `eleaps` (whose output option `$subsets` are matrices or 3-d arrays), using a different criterion (see the example below).

**Value**

The value of the $\zeta^2$ coefficient.

**Examples**

```r
## 1) A Linear Discriminant Analysis example with a very small data set.
## We considered the Iris data and three groups,
## defined by species (setosa, versicolor and virginica).

data(iris)
irisHmat <- ldaHmat(iris[1:4],iris$Species)
zeta2.coef(irisHmat$mat,H=irisHmat$H,r=2,c(1,3))
## [1] 0.9211501

## 2) An example computing the value of the zeta_2 criterion for two
## subsets produced when the anneal function attempted to optimize
## the ccr1_2 criterion (using an absurdly small number of iterations).

ccr1results<-anneal(irisHmat$mat,2,nsol=2,niter=2,criterion="ccr12",
H=irisHmat$H,r=2)
zeta2.coef(irisHmat$mat,H=irisHmat$H,r=2,ccr1results$subsets)
## Card.2
## Solution 1 0.9105021
## Solution 2 0.9161813
```

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