# Package 'ChemometricsWithR'

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**Type** Package

**Title** Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences

**Version** 0.1.13

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**Description** Functions and scripts used in the book ``Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences" by Ron Wehrens, Springer (2011). Data used in the package are available from github.

**URL** https://github.com/rwehrens/CWR

**BugReports** https://github.com/rwehrens/CWR/issues

**Imports** MASS, pls, kohonen, devtools

**Suggests** nnet, randomForest, ada, rrcov, sfsmisc, ipred, fastICA, rda, TIMP, class, e1071, rpart, cluster, ALS, ptw, dtw, boot, leaps, lars, elasticnet, subselect, signal, mclust

**License** GPL (>= 2)

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**NeedsCompilation** no

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## R topics documented:

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`ChemometricsWithR-package` *Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences*

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## Description

Functions and scripts used in the book "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences" by Ron Wehrens, Springer (2011). Data used in the package are available from github.

## Details

The accompanying **ChemometricsWithRData** package (approx. 60 MB) contains a couple of data sets used in the book that are too large for CRAN according to current size limits. For details on how to install the data package, use `?installChemometricsWithRData`.

## Author(s)

Ron Wehrens

Maintainer: Ron Wehrens <ron.wehrens@gmail.com>

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

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`AdjRkl` *Adjusted Rand Index*

---

## Description

The Adjusted Rand Index is a measure of similarity for two groupings or clusterings. A value of 1 indicates total agreement.

## Usage

```
AdjRkl(part1, part2)
```

### Arguments

| | |
|---|---|
| part1 | First partitioning. |
| part2 | Second partitioning. |

### Value

Number.

### Author(s)

Ron Wehrens

### References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

### Examples

```
if (require("kohonen")) {
  data(wines, package = "kohonen")
  wines.dist <- dist(scale(wines))
  wines.sl <- hclust(wines.dist, method = "single")
  wines.cl <- hclust(wines.dist, method = "complete")

  AdjRkl(cutree(wines.sl, 4), cutree(wines.cl, 4))
} else {
  cat("Package kohonen not available.\nInstall it by typing 'install.packages(\"kohonen\")'")
}
```

---

## Error *Often-used error functions*

---

### Description

Error functions for classification and regression

### Usage

```
rms(x, y)
err.rate(x, y)
```

### Arguments

| | |
|---|---|
| x, y | True or predicted values, either numbers or factors. |

## Value

Function `rms` returns the root-mean-square error for real-valued x and y vectors. Function `err.rate` returns the fraction of non-matching cases in x and y (real numbers or factors).

## Author(s)

Ron Wehrens

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

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`Evaluation` *Evaluation function examples for SA- or GA-based variable selection in classification applications.*

---

## Description

Two examples of functions that can be used in variable selection for classification. The outcome of these functions should be maximized by the optimization.

## Usage

```
lda.loofun(x, grouping, subset, ...)
pls.cvfun(x, response, subset, ...)
```

## Arguments

| | |
|---|---|
| `x` | Data matrix: independent variables used by `eval.fun` |
| `grouping` | Class vector, possibly a factor |
| `response` | Dependent variable, typically a real number |
| `subset` | A vector containing the indices of the variables to be included |
| `...` | Further arguments, such as the number of latent variables to use in `plscvfun` |

## Details

The evaluation function should give high values for good subsets, and low values for bad subsets. The `lda.loofun` function simply counts the number of correct predictions in LOO crossvalidation, and subtracts the number of variables in the subset. Function `pls.cvfun` returns the mean squared error of cross-validation.

## Value

One value indicating the quality of the subset

## Author(s)

Ron Wehrens

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

## See Also

GA, SA

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GA *Genetic Algorithms for variable selection in classification*

---

## Description

A set of functions implementing simple variable selection in classification applications using genetic algorithms.

## Usage

```
GAfun(X, C, eval.fun, kmin, kmax, popsize = 20, niter = 50,
      mut.prob = 0.05, ...)
GAfun2(X, C, eval.fun, kmin, kmax, popsize = 20, niter = 50,
       mut.prob = 0.05, ...)

GA.init.pop(popsize, nvar, kmin, kmax)
GA.select(pop, number, qlts, min.qlt = 0.4, qlt.exp = 1)
GA.mut(subset, maxvar, mut.prob = 0.01)
GA.XO(subset1, subset2)
```

## Arguments

| | |
|---|---|
| X | Data matrix: independent variables used by eval.fun |
| C | Class vector, used by eval.fun |
| eval.fun | evaluation function. Should take a data matrix, a class vector (or factor), and a subset argument |
| kmin | Minimal number of variables to retain |
| kmax | Maximal number of variables to retain |
| popsize | Size of the GA population |
| niter | Number of iterations |
| mut.prob | Mutation probability |
| ... | Further arguments to the evaluation function |

| | |
|---|---|
| nvar | The total number of variables to choose from |
| pop, subset, subset1, subset2 | A (part of a) population of trial solutions |
| number | The number of trial solutions that may produce offspring |
| qlts | Vector of quality measures for members in a population |
| min.qlt | Minimal quality of a trial solution to be considered as a future parent |
| qlt.exp | Quality scaling parameter: the larger this number, the more discrimination between good and bad solutions, and the more greedy the search characteristics |
| maxvar | Number of variables to choose from |

## Details

The function generates a population of trial solutions, each containing a number of variables to be retained. For every member of the population, the evaluation function calculates a quality measure, which determines the chance of that member to create offspring. In a process of "survival of the fittest", this leads to subsets for which the evaluation function has a maximal value.

The initialization is done randomly. Selection is simple threshold selection. Mutation swaps variables in or out of the subset; the cross-over type is uniform. Functions `GA.init.pop`, `GA.select`, `GA.mut` and `GA.XO` are auxiliary functions, not meant to be called directly by the user.

## Value

Functions `GAfun` and `GAfun2` both return a list containing the following fields:

| | |
|---|---|
| best | The best subset |
| best.q | The quality of the best subset |
| n.iter | The number of iterations |

In addition, the outcome of `GAfun2` also contains

| | |
|---|---|
| qualities | A matrix containing the best, median and worst quality value throughout the optimization |

## Author(s)

Ron Wehrens

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

## See Also

Evaluation, SA

## Examples

```
if (require("pls")) {
  data(gasoline, package = "pls")
  ## Usually more iterations are needed
  GAobj <- GAfun(gasoline$NIR, gasoline$octane,
                 eval.fun = pls.cvfun, niter = 20,
                 kmin = 3, kmax = 25, ncomp = 2)
  GAobj
} else {
  cat("Package pls not available.\nInstall it by typing 'install.packages(\"pls\")'")
}
```

---

`gini` *Gini impurity index for cart objects*

---

## Description

A simple implementation of the Gini impurity index for classification and regression trees. Not meant to be called directly - included for demonstration purposes.

## Usage

```
gini(x, class, splitpoint)
```

## Arguments

| | |
|---|---|
| `x` | Numeric vector of length n. |
| `class` | Class labels, length n. |
| `splitpoint` | Tentative split point. |

## Value

The Gini impurity index, given a certain split point, a vector of possible splits, and a vector of class labels. Lower values indicate more pure leaves.

## Author(s)

Ron Wehrens

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

installChemometricsWithRData *Installation of ChemometricsWithRData*

## Description

Function to download and install the **ChemometricsWithRData** package from its github location.

## Details

The total size of the data sets in the ChemometricsWithRData package (`Prostate2000Raw`, `prostate`, `bdata` and `shootout`) is too large for CRAN according to current guidelines. The data package is now available from github only.

## Author(s)

Ron Wehrens

Maintainer: Ron Wehrens <ron.wehrens@gmail.com>

## References

Ron Wehrens (2011). Chemometrics With R: Multivariate Data Analysis in the Natural Sciences and Life Sciences. Springer, Heidelberg.

## Examples

```
## Not run:
  installChemometricsWithRData()

## End(Not run)
```

MCR *Functions for Multivariate Curve Resolution*

## Description

Multivariate Curve Resolution, or MCR, decomposes a bilinear matrix into its pure components. A classical example is a matrix consisting of a series of spectral measurements on a mixture of chemicals for following the reaction. At every time point, a spectrum is measured that is a linear combination of the pure spectra. The goal of MCR is to resolve the pure spectra and concentration profiles over time.

## Usage

```
mcr(x, init, what = c("row", "col"), convergence = 1e-08,
    maxit = 50)
opa(x, ncomp)
efa(x, ncomp)
```

## Arguments

| | |
|---|---|
| x | Data matrix |
| init | Initial guess for pure compounds |
| what | Whether the pure compounds are rows or columns of the data matrix |
| convergence | Convergence criterion |
| maxit | Maximal number of iterations |
| ncomp | Number of pure compounds |

## Details

MCR uses repeated application of least-squares regression to find pure profiles and spectra. The method is iterative; both EFA and OPA are methods to provide initial guesses.

## Value

Function mcr returns a list containing

| | |
|---|---|
| C | An estimate of the pure "concentration profiles" |
| S | An estimate of the pure "spectra" |
| resids | The residuals of the final decomposition |
| rms | Root-mean-square values of the individual iterations |

Function opa returns a list containing

| | |
|---|---|
| pure.compounds: | A matrix containing ncomp pure compounds, usually spectra at specific time points |
| selected: | The wavelengths leading to the estimates of the pure concentration profiles |

Function efa returns a list containing

| | |
|---|---|
| pure.compounds: | A matrix containing ncomp pure compounds, usually concentration profiles at specific wavelengths |
| forward: | The development of the singular values of the reduced data matrix when increasing the number of columns in the forward direction |
| backward: | The development of the singular values of the reduced data matrix when increasing the number of columns in the backwarddirection |

Usually, opa and efa are employed in opposite ways: if opa is used to find the "purest" row of a data matrix, one would typically employ efa to find the "purest" column, and vice versa.

### Author(s)

Ron Wehrens

### References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

### Examples

```
## Not run:
if (require("ChemometricsWithRData")) {
  data(bdata, package = "ChemometricsWithRData")
  D1.efa <- efa(bdata$d1, 3)
  matplot(D1.efa$forward, type = "l")
  matplot(D1.efa$backward, type = "l")
  matplot(D1.efa$pure.comp, type = "l")

  D1.opa <- opa(bdata$d1, 3)
  matplot(D1.opa$pure.comp, type = "l")

  D1.mcr.efa <- mcr(bdata$d1, D1.efa$pure.comp, what = "col")
  matplot(D1.mcr.efa$C, type = "l", main = "Concentration profiles")
  matplot(t(D1.mcr.efa$S), type = "l", main = "Pure spectra")
  }

## End(Not run)
```

---

## PCA *Principal Component Analysis*

---

### Description

Functions for PCA: creating a PCA object, extracting variances, scores and loadings for individual PCs, projecting new data in the PC space, and reconstruction using a limited number of PCs.

### Usage

```
PCA(X, warn = TRUE)
## S3 method for class 'PCA'
summary(object, varperc = 90, pc.select = c(1:5,10), ...)
variances(object, npc = maxpc)
## S3 method for class 'PCA'
scores(object, npc = maxpc, ...)
## S3 method for class 'PCA'
loadings(object, npc = maxpc, ...)
reconstruct(object, npc = maxpc)
project(object, npc = maxpc, newdata, ldngs)
```

## Arguments

| | |
|---|---|
| X | a matrix, with each row representing an object. |
| warn | logical, whether or not to give a warning when the data are not mean-centered. |
| object | an object of class "PCA" (see below). |
| varperc | variance threshold in the summary function. |
| ... | extra arguments, e.g., for printing the variance table (digits = ...). |
| pc.select | PCs to be included in the summary function. |
| npc | the number of PCs to be returned. |
| newdata | data (with the same number of variables as the original data) that are to be projected into the space of the first npc PCs. |
| ldngs | loadings to be used; by default the PCA loadings. |

## Value

Function PCA returns an object of class "PCA" with components

| | |
|---|---|
| scores | object weights per PC. |
| loadings | variable weights per PC. |
| var | variance explained per PC. |
| totalvar | The total variance in the data set. |

Function summary.PCA gives a short summary of the PCA model, stating how many PCs are needed to cover a certain percentage of the total variance, and for selected PCs gives the (cumulative) variance explained.

Function variances returns the variances associated with each PC.

Function scores returns the scores associated with each PC.

Function loadings returns the loadings associated with each PC.

Function reconstruct returns the reconstruction of the original data matrix, based on npc PCs.

Function project projects the new data into the subspace spanned by the given loadings. If argument ldngs is given, arguments pcamod and npc are not needed.

## Author(s)

Ron Wehrens

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

## See Also

plot.PCA

## Examples

```
data(wines, package = "kohonen")
wines.PC <- PCA(scale(wines))
```

---

PCA.plot *Principal Component Analysis plotting functions*

---

## Description

Plotting functions for PCA: for scores, loadings, scores and loadings simultaneously (a biplot), and variances (a screeplot, where the log of the explained variance is plotted for each PC).

## Usage

```
## S3 method for class 'PCA'
scoreplot(object, pc = c(1, 2), pcscores = scores(object),
          show.names = FALSE, xlab, ylab, xlim, ylim, ...)
## S3 method for class 'PCA'
loadingplot(object, pc = c(1, 2), pcloadings = loadings(object),
            scalefactor = 1, add = FALSE, show.names = FALSE,
            xlab, ylab, xlim, ylim, col = "blue", min.length =
            0.01, varnames = NULL, ...)
## S3 method for class 'PCA'
biplot(x, pc = c(1,2),
        show.names = c("none", "scores", "loadings", "both"),
        score.col = 1, loading.col = "blue",
        min.length = .01, varnames = NULL, ...)
screeplot(object, type = c("scree", "percentage"), npc, ...)
```

## Arguments

| | |
|---|---|
| x, object | an object of class "PCA" (see below). |
| pc | which PCs to show. |
| pcscores | matrix of scores, by default the scores of the PCA model object. |
| show.names | show names rather than plotting symbols. For loadingplot and scoreplot a logical (default: FALSE), for biplot one of 'scores', 'loadings', 'both' or 'none' (default). |
| xlab, ylab, xlim, ylim, col | graphical parameters of the plot. |
| pcloadings | matrix of loadings, by default the loadings of the PCA model object. |
| scalefactor | scaling factor for the loadings; used internally, when the loadingplot function is called from within biplot.PCA. |
| add | logical, whether to add to the existing plot (again, useful when loadingplot is called from within biplot.PCA). |

| | |
|---|---|
| npc | how many PCs to show in the scree plot (starting from 1). |
| type | show a real screeplot (scree) or show the percentage of variance explained (percentage). |
| score.col, loading.col | colours of the scores and loadings in a biplot. |
| min.length | minimal length of loading vectors to be plotted by arrows. Vectors that are too short lead to warning messages, are not interesting, and only clutter the graphic. |
| varnames | alternative vector of variable names. |
| ... | Graphical arguments passed on to lower-level plotting functions. |

## Details

Score plots and loading plots show the amount of explained variance at the axis labels only when PCA has been performed at mean-centered data.

## Author(s)

Ron Wehrens

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

## See Also

PCA

## Examples

```
data(wines, package = "kohonen")
wines.PC <- PCA(scale(wines))
wine.classes <- as.integer(vintages)
scoreplot(wines.PC, col = wine.classes, pch = wine.classes)
loadingplot(wines.PC, show.names = TRUE)
biplot(wines.PC, score.col = wine.classes)
screeplot(wines.PC)
```

---

# pick.peaks *Peak-picking function.*

---

## Description

Function to identify local maxima in a vector, typically a spectrum or a chromatogram.

## Usage

```
pick.peaks(x, span)
```

## Arguments

| | |
|---|---|
| x | Numerical vector. |
| span | Neighbourhood, used to define local maxima. |

## Value

A vector containing positions of local maxima in the input data.

## Author(s)

Ron Wehrens

## Examples

```
if (require("ptw")) {
data(lcms, package = "ptw")
plot(lcms[1,,1], type = "l", xlim = c(1000, 1500))
abline(v = pick.peaks(lcms[1,,1], 20), col = "blue")
} else {
  cat("Package ptw not available.\nInstall it by typing 'install.packages(\"ptw\")'")
}
```

---

# SA *Simulated Annealing for variable selection in classification*

---

## Description

A set of functions implementing simple variable selection in classification applications using simulated annealing

## Usage

```
SAfun(x, response, eval.fun, Tinit, niter = 100,
      cooling = 0.05, fraction = 0.3, ...)
SAfun2(x, response, eval.fun, Tinit, niter = 100,
       cooling = 0.05, fraction = 0.3, ...)

SAstep(curr.set, maxvar, fraction = .3, size.dev = 1)
```

## Arguments

| | |
|---|---|
| x | Data matrix: independent variables used by `eval.fun` |
| response | Class vector, used by `eval.fun` |
| eval.fun | evaluation function. Should take a data matrix, a class vector (or factor), and a subset argument |
| Tinit | Initial temperature |

| | |
|---|---|
| niter | Maximal number of iterations |
| cooling | Cooling speed |
| fraction | Size of the desired subset, as a fraction of the total number of variables |
| ... | Further arguments to the evaluation function |
| curr.set | Current trial solution |
| maxvar | The total number of variables to choose from |
| size.dev | Parameter governing the variability in size of subsequent subsets |

## Details

Simulated Annealing (SA) starts with a random subset, and proceeds by random moves in the solution space. In this implementation, a new solution may deviate in length at most size.dev variables: at most two variables may be swapped in or out at each step. If a step is an improvement, it is unconditionally accepted. If not, acceptance is a stochastic process depending on the current temperature - with high temperatures, "bad" moves are more likely to be accepted than with low temperatures. The process stops after a predefined number of iterations.

## Value

Functions SAfun and SAfun2 both return a list containing the following fields:

| | |
|---|---|
| best | The best subset |
| best.q | The quality of the best subset |

In addition, the outcome of SAfun2 also contains

| | |
|---|---|
| qualities | A vector containing quality values of solutions seen throughout the optimization |
| accepts | A vector containing logicals indicating which solutions were accepted and which were rejected |

## Author(s)

Ron Wehrens

## References

R. Wehrens. "Chemometrics with R - Multivariate Data Analysis in the Natural Sciences and Life Sciences". Springer, Heidelberg, 2011.

## See Also

Evaluation, GA

## Examples

```
if (require("pls")) {
data(gasoline, package = "pls")
## usually more than 50 iterations are needed
SAobj <- SAfun(gasoline$NIR, gasoline$octane,
               eval.fun = pls.cvfun, Tinit = 3,
               fraction = .02, niter = 50, ncomp = 2)
SAobj
} else {
  cat("Package pls not available.\nInstall it by typing 'install.packages(\"pls\")'")
}
```

---

`unsigned.range` *Unsigned range of the data vector including zero.*

---

## Description

Function returning the range of the data where, if necessary, the range is extended to include zero. Not meant to be called directly by the user.

## Usage

```
unsigned.range(x)
```

## Arguments

| | |
|---|---|
| x | Numeric vector. |

## Value

A vector of two numbers.

## Note

From the R stats package (see biplot.default).

# Index