

# Package ‘baseline’

September 12, 2020

**Encoding** UTF-8

**Type** Package

**Title** Baseline Correction of Spectra

**Version** 1.3-1

**Date** 2020-09-10

**Maintainer** Kristian Hovde Liland <kristian.liland@nmbu.no>

**Description** Collection of baseline correction algorithms, along with a framework and a Tcl/Tk enabled GUI for optimising baseline algorithm parameters. Typical use of the package is for removing background effects from spectra originating from various types of spectroscopy and spectrometry, possibly optimizing this with regard to regression or classification results. Correction methods include polynomial fitting, weighted local smoothers and many more.

**License** GPL-2

**Depends** R (>= 2.15)

**Imports** graphics, SparseM, grDevices, stats, methods, limSolve

**Suggests** gWidgets2, gWidgets2tcltk, IDPmisc, lattice, pls, MASS

**LazyLoad** true

**LazyData** true

**ZipData** true

**NeedsCompilation** no

**Author** Kristian Hovde Liland [aut, cre],  
Bjørn-Helge Mevik [aut],  
Roberto Canteri [ctb]

**Repository** CRAN

**Date/Publication** 2020-09-12 06:20:03 UTC

## R topics documented:

baseline-package	3
algorithm	4
baseline	5

baseline-class	6
baseline.als	7
baseline.fillPeaks	8
baseline.irls	9
baseline.lowpass	10
baseline.medianWindow	11
baseline.modpolyfit	12
baseline.peakDetection	13
baseline.rfbaseline	14
baseline.rollingBall	16
baseline.shirley	17
baseline.TAP	19
baselineAlg-class	21
baselineAlgorithms	22
baselineAlgorithmsGUI	23
baselineAlgResult-class	23
baselineAlgTest-class	24
baselineEnv	25
baselineGUI	26
custom.baseline	27
doOptim	28
funcName	29
getBaseline	30
ind.min	31
milk	32
name	32
optimWizard	33
overall.min	34
param	35
param.ind.min	35
plotBaseline	36
plotOptim	37
PLSRTest-class	38
predictionResult-class	39
predictionTest-class	40
qualMeas	40
ridgeRegressionTest-class	41
runTest	42
XPSdata	43

---

baseline-package      *Baseline correction*

---

## Description

A common framework with implementations of several baseline correction methods

## Details

Package: baseline  
Type: Package  
Version: 1.2-2  
Date: 2019-11-05  
License: GPL-2

Use function `baseline` for baseline correction. This function takes matrices of spectra, a method name and parameters needed for the specific method. See helpfiles for details.

## Author(s)

Kristian Hovde Liland and Bjørn-Helge Mevik

Maintainer: Kristian Hovde Liland <kristian.liland@nmbu.no>

## References

Andreas F. Ruckstuhl, Matthew P. Jacobson, Robert W. Field, James A. Dodd: Baseline subtraction using robust local regression estimation; CHAD A. LIEBER and ANITA MAHADEVAN-JANSEN: Automated Method for Subtraction of Fluorescence from Biological Raman Spectra; Mark S. Friedrichs: A model-free algorithm for the removal of baseline artifacts; AHMET K. ATAKAN, W. E. BLASS, and D. E. JENNINGS: Elimination of Baseline Variations from a Recorded Spectrum by Ultra-low Frequency Filtering; M.A. Kneen, H.J. Annegarn: Algorithm for fitting XRF, SEM and PIXE X-ray spectra backgrounds; K.H. Liland, B.-H. Mevik, E.-O. Rukke, T. Almøy, M. Skaugen and T. Isaksson (2009) Quantitative whole spectrum analysis with MALDI-TOF MS, Part I: Measurement optimisation. *Chemometrics and Intelligent Laboratory Systems*, **96**(2), 210–218.

## Examples

```
# Load data
data(milk)
# The baseline() function is an S4 wrapper for all the different
# baseline correction methods. The default correction method
# is IRLS. Data must be organized as row vectors in a matrix
# or data.frame.
bc.irls <- baseline(milk$spectra[1,, drop=FALSE])
## Not run:
# Computationally heavy
```

```
plot(bc.irls)

## End(Not run)

# Available extractors are:
# getBaseline(bc.irls)
# getSpectra(bc.irls)
# getCorrected(bc.irls)
# getCall(bc.irls)

# Correction methods and parameters can be specified through the wrapper.
bc.fillPeaks <- baseline(milk$spectra[1,, drop=FALSE], lambda=6,
hwi=50, it=10, int=2000, method='fillPeaks')
## Not run:
# Computationally heavy
plot(bc.fillPeaks)

## End(Not run)

# If a suitable gWidgets2 implementation is installed, a
# graphical user interface is available for interactive
# parameter adaption.
## Not run:
# Dependent on external software
baselineGUI(milk$spectra)

## End(Not run)
```

---

algorithm

*Extraction methods for "baselineAlgTest" objects*

---

## Description

Extraction methods specifically for objects of class `baselineAlgTest`

## Usage

```
algorithm(object)
extraArgs(object)
```

## Arguments

object            Object of class `baselineAlgTest`

## Value

The corresponding slot

## Author(s)

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

[baselineAlgTest](#)

---

baseline

*Baseline correction*

---

**Description**

Common framework for baseline correction

**Usage**

```
baseline(spectra, method = "irls", ...)
```

**Arguments**

spectra	Matrix with spectra in rows
method	Baseline correction method
...	Additional parameters, sent to the method

**Details**

Estimates baselines for the spectra, using the algorithm named in method.

**Value**

An object of class [baseline](#).

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

Kristian Hovde Liland, Trygve Almøy, Bjørn-Helge Mevik (2010), Optimal Choice of Baseline Correction for Multivariate Calibration of Spectra, *Applied Spectroscopy* 64, pp. 1007-1016.

**See Also**

The functions implementing the baseline algorithms: [baseline.als](#), [baseline.fillPeaks](#), [baseline.irls](#), [baseline.lowpass](#), [baseline.medianWindow](#), [baseline.modpolyfit](#), [baseline.peakDetection](#), [baseline.rfbaseline](#), [baseline.rollingBall](#), [baseline.shirley](#), [baseline.TAP](#)

**Examples**

```

# Load data
data(milk)
# The baseline() function is an S4 wrapper for all the different
# baseline correction methods. The default correction method
# is IRLS. Data must be organized as row vectors in a matrix
# or data.frame.
bc.irls <- baseline(milk$spectra[1,, drop=FALSE])
## Not run:
  # Computationally heavy
plot(bc.irls)

## End(Not run)

# Available extractors are:
# getBaseline(bc.irls)
# getSpectra(bc.irls)
# getCorrected(bc.irls)
# getCall(bc.irls)

# Correction methods and parameters can be specified through the wrapper.
bc.fillPeaks <- baseline(milk$spectra[1,, drop=FALSE], lambda=6,
hwi=50, it=10, int=2000, method='fillPeaks')
## Not run:
  # Computationally heavy
plot(bc.fillPeaks)

## End(Not run)

# If a suitable gWidgets2 implementation is installed, a
# graphical user interface is available for interactive
# parameter adaption.
## Not run:
  # Dependent on external software
  baselineGUI(milk$spectra)

## End(Not run)

```

---

baseline-class

Class "baseline"

---

**Description**

Stores the result of estimating baselines for one or more spectra.

**Objects from the Class**

The normal way to create objects is with the function [baseline](#). Several baseline algorithms are available. See [baseline](#) for details. There is a plot method for the class; see [plot, baseline-method](#).

**Slots**

**baseline:** A matrix with the estimated baselines

**corrected:** A matrix with the corrected spectra

**spectra:** A matrix with the original spectra

**call:** The call to [baseline](#)

**Methods**

**getBaseline** signature(object = "baseline"): Extract the estimated baselines

**getCall** signature(object = "baseline"): Extract the call to [baseline](#) used to create the object

**getCorrected** signature(object = "baseline"): Extract the corrected spectra

**getSpectra** signature(object = "baseline"): Extract the original spectra

**Warning**

In a future version, one of the slots might be removed from the class definition and calculated on the fly instead, in order to save space. Therefore, *do* use the extractor functions (`getSpectra`, `getBaseline` and `getCorrected`) instead of accessing the slots directly.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

[baseline](#), [getBaseline](#), [getSpectra](#), [getCorrected](#), [getCall](#)

**Examples**

```
showClass("baseline")
```

---

baseline.als

*Asymmetric Least Squares*

---

**Description**

Baseline correction by 2nd derivative constrained weighted regression. Original algorithm proposed by Paul H. C. Eilers and Hans F.M. Boelens

**Usage**

```
baseline.als(spectra, lambda = 6, p = 0.05, maxit = 20)
```

**Arguments**

spectra	Matrix with spectra in rows
lambda	2nd derivative constraint
p	Weighting of positive residuals
maxit	Maximum number of iterations

**Details**

Iterative algorithm applying 2nd derivative constraints. Weights from previous iteration is p for positive residuals and 1-p for negative residuals.

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra
wgts	Matrix of final regression weights

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

Paul H. C. Eilers and Hans F.M. Boelens: Baseline Correction with Asymmetric Least Squares Smoothing

**Examples**

```
data(milk)
bc.als <- baseline(milk$spectra[1,, drop=FALSE], lambda=10, method='als')
## Not run:
plot(bc.als)

## End(Not run)
```

---

baseline.fillPeaks      *Fill peaks*

---

**Description**

An iterative algorithm using suppression of baseline by means in local windows

**Usage**

```
baseline.fillPeaks(spectra, lambda, hwi, it, int)
```



**Arguments**

spectra	Matrix with spectra in rows
lambda	2nd derivative penalty for primary smoothing
hwi	Half width of local windows
it	Number of iterations in suppression loop
int	Number of buckets to divide spectra into

**Details**

In local windows of buckets the minimum of the mean and the previous iteration is chosen as the new baseline

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

Kristian Hovde Liland, 4S Peak Filling - baseline estimation by iterative mean suppression, MethodsX 2015

**Examples**

```
data(milk)
bc.fillPeaks <- baseline(milk$spectra[1,, drop=FALSE], lambda=6,
hwi=50, it=10, int=2000, method='fillPeaks')
## Not run:
plot(bc.fillPeaks)

## End(Not run)
```

---

baseline.irls

*Iterative Restricted Least Squares*


---

**Description**

An algorithm with primary smoothing and repeated baseline suppressions and regressions with 2nd derivative constraint

**Usage**

```
baseline.irls(spectra, lambda1 = 5, lambda2 = 9, maxit = 200, wi = 0.05)
```

**Arguments**

spectra	Matrix with spectra in rows
lambda1	2nd derivative constraint for primary smoothing
lambda2	2nd derivative constraint for secondary smoothing
maxit	Maximum number of iterations
wi	Weighting of positive residuals

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra
smoothed	Matrix of primary smoothed spectra

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**Examples**

```
data(milk)
bc.irls <- baseline(milk$spectra[1,, drop=FALSE], method='irls')
## Not run:
plot(bc.irls)

## End(Not run)
```

---

baseline.lowpass      *Low-pass FFT filter*

---

**Description**

An algorithm for removing baselines based on Fast Fourier Transform filtering

**Usage**

```
baseline.lowpass(spectra, steep = 2, half = 5)
```

**Arguments**

spectra	Matrix with spectra in rows
steep	Steepness of filter curve
half	Half-way point of filter curve

**Details**

Since the scale of the spectra will be different after filtering, baselines will not be returned by the algorithm

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

AHMET K. ATAKAN, W. E. BLASS, and D. E. JENNINGS: Elimination of Baseline Variations from a Recorded Spectrum by Ultra-low Frequency Filtering

**Examples**

```
data(milk)
bc.lowpass <- baseline(milk$spectra[1,, drop=FALSE], method='lowpass')
## Not run:
plot(bc.lowpass)

## End(Not run)
```

---

baseline.medianWindow *Median window*

---

**Description**

An implementation and extention of Mark S. Friedrichs' model-free algorithm

**Usage**

```
baseline.medianWindow(spectra, hwm, hws, end)
```

**Arguments**

spectra	Matrix with spectra in rows
hwm	Window half width for local medians
hws	Window half width for local smoothing (optional)
end	Original endpoint handling (optional boolean)

**Details**

An algorithm finding medians in local windows and smoothing with gaussian weighting

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

Mark S. Friedrichs: A model-free algorithm for the removal of baseline artifacts

**Examples**

```
data(milk)
bc.medianWindow <- baseline(milk$spectra[1,, drop=FALSE], hwm=300,
method='medianWindow')
## Not run:
plot(bc.medianWindow)

## End(Not run)
```

---

baseline.modpolyfit    *Modified polynomial fitting*

---

**Description**

An implementation of CHAD A. LIEBER and ANITA MAHADEVAN-JANSENs algorithm for polynomial fitting

**Usage**

```
baseline.modpolyfit(spectra, t, degree = 4, tol = 0.001, rep = 100)
```

**Arguments**

spectra	Matrix with spectra in rows
t	Optional vector of spectrum abscissa
degree	Degree of polynomial
tol	Tolerance of difference between iterations
rep	Maximum number of iterations

**Details**

Polynomial fitting with baseline suppression relative to original spectrum

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

CHAD A. LIEBER and ANITA MAHADEVAN-JANSEN: Automated Method for Subtraction of Fluorescence from Biological Raman Spectra

**Examples**

```
data(milk)
bc.modpolyfit <- baseline(milk$spectra[1,, drop=FALSE], method='modpolyfit', deg=6)
## Not run:
plot(bc.modpolyfit)

## End(Not run)
```

---

baseline.peakDetection

*Simultaneous Peak Detection and Baseline Correction*

---

**Description**

A translation from Kevin R. Coombes et al.'s MATLAB code for detecting peaks and removing baselines

**Usage**

```
baseline.peakDetection(spectra, left, right, lwin, rwin, snminimum,
mono=0, multiplier=5, left.right, lwin.rwin)
```

**Arguments**

spectra	Matrix with spectra in rows
left	Smallest window size for peak widths
right	Largest window size for peak widths
lwin	Smallest window size for minimums and medians in peak removed spectra
rwin	Largest window size for minimums and medians in peak removed spectra
snminimum	Minimum signal to noise ratio for accepting peaks
mono	Monotonically decreasing baseline if mono>0
multiplier	Internal window size multiplier
left.right	Sets left and right to value of left.right
lwin.rwin	Sets lwin and rwin to value of lwin.rwin

**Details**

Peak detection is done in several steps sorting out real peaks through different criteria. Peaks are removed from spectra and minimums and medians are used to smooth the remaining parts of the spectra. If `snminimum` is omitted, `y3`, `midspec`, `y` and `y2` are not returned (faster)

**Value**

<code>baseline</code>	Matrix of baselines corresponding to spectra <code>spectra</code>
<code>corrected</code>	Matrix of baseline corrected spectra
<code>peaks</code>	Final list of selected peaks
<code>sn</code>	List signal to noise ratios for peaks
<code>y3</code>	List of peaks prior to signal to noise selection
<code>midspec</code>	Mid-way baseline estimation
<code>y</code>	First estimate of peaks
<code>y2</code>	Second estimate of peaks

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

KEVIN R. COOMBES et al.: Quality control and peak finding for proteomics data collected from nipple aspirate fluid by surface-enhanced laser desorption and ionization.

**Examples**

```
data(milk)
bc.peakDetection <- baseline(milk$spectra[1,, drop=FALSE], method='peakDetection',
left=300, right=300, lwin=50, rwin=50)
## Not run:
plot(bc.peakDetection)

## End(Not run)
```

---

baseline.rfbaseline     *Robust Baseline Estimation*

---

**Description**

Wrapper for Andreas F. Ruckstuhl, Matthew P. Jacobson, Robert W. Field, James A. Dodd's algorithm based on LOWESS and weighted regression

**Usage**

```
baseline.rfbaseline(spectra, span = 2/3, NoXP = NULL, maxit = c(2, 2),
  b = 3.5, weight = NULL, Scale = function(r) median(abs(r))/0.6745,
  delta = NULL, SORT = FALSE, DOT = FALSE, init = NULL)
```

**Arguments**

spectra	Matrix with spectra in rows
span	Amount of smoothing (by fraction of points)
NoXP	Amount of smoothing (by number of points)
maxit	Maximum number of iterations in robust fit
b	Tuning constant in the biweight function
weight	Optional weights to be given to individual observations
Scale	S function specifying how to calculate the scale of the residuals
delta	Nonnegative parameter which may be used to save computation. (See rfbaseline)
SORT	Boolean variable indicating whether x data must be sorted.
DOT	Disregard outliers totally (boolean)
init	Values of initial fit

**Details**

Most of the code is the original code as given by the authors. The ability to sort by X-values has been removed and ability to handle multiple spectra has been added

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**References**

Andreas F. Ruckstuhl, Matthew P. Jacobson, Robert W. Field, James A. Dodd: Baseline subtraction using robust local regression estimation

**Examples**

```
data(milk)
bc.rbe <- baseline(milk$spectra[1,, drop=FALSE], method='rfbaseline',
  span=NULL, NoXP=1000)
## Not run:
plot(bc.rbe)

## End(Not run)
```

---

baseline.rollingBall    *Rolling ball*

---

### Description

Ideas from Rolling Ball algorithm for X-ray spectra by M.A.Kneen and H.J. Annegarn. Variable window width has been left out

### Usage

```
baseline.rollingBall(spectra, wm, ws)
```

### Arguments

spectra	Matrix with spectra in rows
wm	Width of local window for minimization/maximization
ws	Width of local window for smoothing

### Value

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra

### Author(s)

Kristian Hovde Liland and Bjørn-Helge Mevik

### References

M.A. Kneen, H.J. Annegarn: Algorithm for fitting XRF, SEM and PIXE X-ray spectra backgrounds

### Examples

```
data(milk)
bc.rollingBall <- baseline(milk$spectra[1,, drop=FALSE], wm=200, ws=200,
method='rollingBall')
## Not run:
plot(bc.rollingBall)

## End(Not run)
```



---

baseline.shirley      *Shirley Background Estimation*

---

### Description

Shirley Background correction for X-ray Photoelectron Spectroscopy.

### Usage

```
baseline.shirley(spectra, t = NULL, limits = NULL, maxit = 50, err = 1e-6)
```

### Arguments

spectra	matrix with only 1 y-coordinates by rows (i.e.: y = spectra[1,])
t	Optional vector of spectrum abscissa
limits	list with the y coordinates between calculation of background. Ususally these are the extreme point of the data range.
maxit	max number of iteration
err	Tolerance of difference between iterations

### Details

The shape of the spectrum background or baseline is affected by inelastic energy loss processes, secondary electrons and nearby peaks. A reasonable approximation is essential for a qualitative and quantitative analysis of XPS data especially if several components interfere in one spectrum. The choice of an adequate background model is determined by the physical and chemical conditions of the measurements and the significance of the background to the information to be obtained. The subtraction of the baseline before entering the fit iterations or the calculation of the peak area can be an acceptable approximation for simple analytical problems. In order to obtain chemical and physical parameters in detail, however, it is absolutely necessary to include the background function in the iterative peak fit procedure. The primary function  $F(E)$  results from the experimentally obtained function  $M(E)$  and the background function  $U(E)$  as

$$F(E) = M(E) - U(E)$$

The kinetic energy  $E$  of the spectra can be described as

$$E = SE + SW * (i - 1)$$

SE means the start energy in eV, SW is the step width in eV and  $i$  the channel number.  $i$  can assume values between 1 and  $N$  with  $N$  as the number of data points.

In case of baseline calculation before initiating the fit procedure, the background is set to the averaged experimental function  $M(E)$  in a sector around the chosen start and end channels. With  $i_1$  as left channel ( $E_1$ : low energy side) and  $i_2$  as right channel ( $E_2$ : high energy side) the simulation of the baseline is obtained as

$$U(E_1) = M(E_1)$$

and

$$U(E_2) = M(E_2)$$

If ZAP is the number of points used for averaging (can be set in the preferences), the intensity of the averaged measuring function at the low energy side is calculated by

$$M(i_1) = \frac{\sum_{i=0}^{ZAP-1} M(i_1 + i)}{ZAP}$$

and at the high energy side by

$$M(i_2) = \frac{\sum_{i=0}^{ZAP-1} M(i_2 + i)}{ZAP}$$

In many cases the Shirley model turned out to be a successful approximation for the inelastic background of core level peaks of buried species, which suffered significantly from inelastic losses of the emitted photoelectrons. The calculation of the baseline is an iterative procedure. The number of iteration cycles should be chosen high enough so that the shape of the obtained background function does not change anymore. The analytical expression for the Shirley background is

$$U(E) = \int_E^{\infty} F(E') dE' + c$$

The algorithm of Proctor and Sherwood ([1] A. Proctor, P.M.A. Sherwood, Anal. Chem. 54 (1982) 13) is based on the assumption that for every point of the spectrum the background intensity generated by a photoelectron line is proportional to the number of all photoelectrons with higher kinetic energy. The intensity of the background U(i) in channel i is given by

$$U(i) = \frac{(a - b)Q(i)}{P(i) + Q(i)} + b$$

where a and b are the measured intensities in channel  $i_1$  and  $i_2$ , respectively, and P(i) and Q(i) represent the effective peak areas to lower and higher kinetic energies relative to the channel under consideration. An iterative procedure is necessary because P, Q, and U(i) are unknown. In first approximation U(i) = b is used.

The function `baseline.shirley` implements the shirley baseline. It is an iterative algorithm. The iteration stops when the deviation between two consequent iteration is lower than `err` or when the max number of iterations `maxit` is reached.

## Value

The baseline function return an object of class `baseline`.

## References

A. Proctor, P.M.A. Sherwood, Anal. Chem. 54 (1982) 13.

## See Also

[baseline](#)

## Examples

```
data("01s")
Data <- 01s

## The same example with C1s data
# data("C1s")
# Data <- C1s

Y <- Data[2,, drop = FALSE]
X <- Data[1,]

corrected <- baseline(Y, method = "shirley", t = X)
plot(corrected, rev.x = TRUE, labels = X)

## Not run:
# Dependent on external software
baselineGUI(Y, labels=X, method="shirley")

## End(Not run)
```

---

baseline.TAP

*TAP*

---

## Description

An implementation of Roman Svoboda and Jirí Málek's algorithm for baseline identification in kinetic analysis of derivative kinetic data.

## Usage

```
baseline.TAP(spectra, t, interval = 15, tol = 0.001)
```

## Arguments

spectra	Matrix with spectra in rows
t	Optional vector of spectrum abscissa
interval	Distance from spectrum end to starting points for the TAP (default = 15)
tol	Tolerance of difference between iterations (default = 0.001)

**Details**

(i) A first approximation of the baseline equation is selected as the straight line between start and end of the curve. (ii) Based on the first approximation of the baseline equation, the phase change progress parameter is calculated. (iii) An updated equation of the baseline is calculated and the phase change progress parameter equation from step (ii). (iv) The baseline equation from step (iii) is compared (point by point) with the one from the previous iteration. If the convergence criterion is met (the difference between every baseline value corresponding to two successive iterations was less than 0.1%) the procedure is stopped and the final baseline equation is selected. If the convergence criterion is not fulfilled then a new iteration is carried out from step (ii) until convergence was achieved.

**Value**

baseline	Matrix of baselines corresponding to spectra spectra
corrected	Matrix of baseline corrected spectra

**Author(s)**

Kristian Hovde Liland

**References**

Roman Svoboda and Jirí Málek: Importance of proper baseline identification for the subsequent kinetic analysis of derivative kinetic data, Journal of Thermal Analysis and Calorimetry.

**Examples**

```
# My T
myT <- 40:170

# My artificial curve
myAlpha <- c(seq(0.01, 0.02, length.out=40),
             dnorm(seq(-3,3,length.out=51))/2+(0:50)/2000+0.02)
myAlpha <- c(myAlpha,
             seq(myAlpha[90]-0.001, 0.01, length.out=40))
myAlpha <- myAlpha - min(myAlpha)
myAlpha <- cumsum(dadt <- myAlpha/sum(myAlpha))

# Discrete derivative
mydAlpha <- c(0,diff(myAlpha)); mydAlpha <- matrix(mydAlpha, ncol=length(mydAlpha))
rm(myAlpha) # Throw away myAlpha

# Compute baseline from T and derivative
B <- baseline(mydAlpha, t=myT, method="TAP")

# Plot
plot(B, xlab = "T", ylab = "da/dT")
```

---

baselineAlg-class	Class "baselineAlg"
-------------------	---------------------

---

### Description

A class that describes a baseline correction algorithm. The idea is that it contains all information needed to use an algorithm with the optimisation framework and the graphical user interface (but see Notes below).

### Objects from the Class

Objects can be created by calls of the form `new("baselineAlg", ...)`.

### Slots

**name:** Short-name of the algorithm. This must match the name of the object in the `baselineAlgorithms` list of algorithms, and is used throughout the code to identify the algorithm. It should thus start with a letter and contain only letters, digits, underscores ("`_`") or dots ("`.`").

**description:** Description of the algorithm, typically the full name. This will be used in the code to describe the algorithm, so it should not be too long, and not contain newline characters.

**funcName:** The name of the function used to estimate the baseline. The function must take an argument `spectra`, and return a list with the estimated baselines (`baseline`) original spectra (`spectra`) and the corrected spectra (`corrected`). It can also take other arguments (typically parameters) and return additional components in the list.

**param:** A data frame with information about the parameters of the algorithm. It should contain the following columns: `name` - the name of the parameter; `integer` - TRUE if the parameter only takes integer values, otherwise FALSE; `min` - the lower limit of allowed values; `incl.min` - TRUE if the lower limit is an allowed value, otherwise FALSE; `default` - the default value; `max` - the upper limit of allowed values; `incl.max` - TRUE if the upper limit is an allowed value, otherwise FALSE

### Methods

**description** signature(object = "baselineAlg"): Extract the description slot

**funcName** signature(object = "baselineAlg"): Extract the funcName slot

**name** signature(object = "baselineAlg"): Extract the name slot

**param** signature(object = "baselineAlg"): Extract the param slot

### Note

The goal is that the optimisation framework and the GUI code should get all information about available baseline algorithms through a list of `baselineAlg` objects. This will make it relatively simple to add new baseline algorithms.

Currently, there is information about the algorithms spread around in the code. We plan to move that information into the `baselineAlg` objects, and expand the class accordingly.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**Examples**

```
showClass("baselineAlg")
```

---

baselineAlgorithms      *List of available baseline algorithms*

---

**Description**

A list with descriptions of all baseline algorithms available through the optimisaion framework and graphical user interface. The elements of the list are `baselineAlg` objects. The list is used by the code to extract names and information about the baseline algorithms.

**Details**

The list is not meant for usage by end-users, but is extendable and customizable, allowing for extra algorithms or removal of algorithms.

The names of the list must match the name slot of the elements.

**Examples**

```
## Get a list of all algorithms:
names(baselineAlgorithms)
## Show the descriptions
sapply(baselineAlgorithms, description)
## Add new algorithm
baseline.my.alg <- function(spectra, kappa=1, gamma=1){
  baseline <- spectra-kappa+gamma
  corrected <- spectra-baseline
  list(baseline=baseline,corrected=corrected)
}

baselineAlgorithms$my.alg = new("baselineAlg",
  name = "my.alg",
  description = "A new baseline correction algorithm",
  funcName = "baseline.my.alg",
  param = data.frame(
    name = c("kappa","gamma"), # maxit
    integer = c(FALSE, FALSE),
    min = c(0, 0),
    incl.min = c(TRUE, TRUE),
    default = c(1, 1),
    max = c(Inf, 1),
    incl.max = c(FALSE, TRUE)
  ))
```

---

baselineAlgorithmsGUI *List of available baseline algorithms for GUI function*

---

### Description

A list with data.frames containing parameters, minimum and maximum values for GUIs, step lengths for sliders, default values and currently selected values, plus a short description of each parameter. The list is used by the GUIs, and is user customizable.

### Details

The list is not meant for usage by end-users, but is extendable and customizable, allowing for extra algorithms, removal of algorithms or changing of parameter sets.

### Examples

```
## Get a list of all algorithms:
names(baselineAlgorithmsGUI)
## Add new algorithm:
baselineAlgorithmsGUI$my.alg <- as.data.frame(matrix(c(0,20,1,1, 0,20,1,1), 2,4, byrow=TRUE))
dimnames(baselineAlgorithmsGUI$my.alg) <- list(par=c("kappa", "gamma"),
val=c("min", "max", "step", "default"))
baselineAlgorithmsGUI$my.alg$current <- c(1,1)
baselineAlgorithmsGUI$my.alg$name <- c("Subtractive constant", "Additive constant")
```

---

baselineAlgResult-class  
*Class "baselineAlgResult"*

---

### Description

A class describing the result of a baseline algorithm test

### Objects from the Class

Objects are typically created by running `runTest` on a `baselineAlgTest` object.

### Slots

**param:** A named list with the parameter values that were tested. This includes both the predictor parameters and the baseline algorithm parameters. All combinations of values are tested.

**qualMeas:** A matrix of quality measure values for the different combinations of parameter values. Each row corresponds to one prediction parameter value, and each column to one combination of baseline parameters.

**qualMeas.ind.min:** The index in `qualMeas` of the minimum quality measure value

**minQualMeas:** The minimum quality measure value  
**param.ind.min:** A vector of indices into the elements of param of the parameter values corresponding to the minimum quality measure value  
**param.min:** A list of the parameter values corresponding to the minimum quality measure value  
**qualMeasName:** The name of the quality measure

### Methods

**minQualMeas** signature(object = "baselineAlgResult"): Extract the minQualMeas slot  
**param** signature(object = "baselineAlgResult"): Extract the param slot  
**param.ind.min** signature(object = "baselineAlgResult"): Extract the param.ind.min slot  
**param.min** signature(object = "baselineAlgResult"): Extract the param.min slot  
**qualMeas** signature(object = "baselineAlgResult"): Extract the qualMeas slot  
**qualMeas.ind.min** signature(object = "baselineAlgResult"): Extract the qualMeas.ind.min slot  
**qualMeasName** signature(object = "baselineAlgResult"): Extract the qualMeasName slot

### Author(s)

Bjørn-Helge Mevik and Kristian Hovde Liland

### See Also

Class [baselineAlgTest](#), function `runTest`.

### Examples

```
showClass("baselineAlgResult")
```

---

```
baselineAlgTest-class Class "baselineAlgTest"
```

---

### Description

A class that describes a baseline algorithm test. The test is performed with the function `runTest`.

### Objects from the Class

Objects can be created by calls of the form `new("baselineAlgTest", ...)`.

### Slots

**algorithm:** A "baselineAlg" object. The baseline algorithm to test.  
**param:** A named list with parameter values to test. All combinations of parameters are tested.  
**extraArgs:** A named list of extra parameters to the baseline algorithm. These will be held fixed during the testing.



**Methods**

**algorithm** signature(object = "baselineAlgTest"): Extract the algorithm slot  
**extraArgs** signature(object = "baselineAlgTest"): Extract the extraArgs slot ...  
**funcName** signature(object = "baselineAlgTest"): Extract the funcName slot ...  
**param** signature(object = "baselineAlgTest"): Extract the param slot  
**runTest** signature(object = "baselineAlgTest"): Run the test.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

Classes [baselineAlg](#), [baselineAlgResult](#). Function [runTest](#).

**Examples**

```
showClass("baselineAlgTest")
```

---

baselineEnv

*Baseline environment*

---

**Description**

Methods to access the baseline environment.

**Usage**

```
baselineEnv()  
getBaselineEnv(x, mode="any")  
putBaselineEnv(x, value)
```

**Arguments**

x	Name of object to put/get.
mode	Mode of object to get.
value	Object to put.

**Value**

getBaseline retrieves an object.

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

### See Also

The functions implementing the baseline algorithms: [baseline.als](#), [baseline.fillPeaks](#), [baseline.irls](#), [baseline.lowpass](#), [baseline.medianWindow](#), [baseline.modpolyfit](#), [baseline.peakDetection](#), [baseline.rfbaseline](#), [baseline.rollingBall](#)

### Examples

```
putBaselineEnv('fish', '<==x-<')
getBaselineEnv('fish')
```

---

baselineGUI

*Interactive plotting tool*

---

### Description

An interactive plotting tool for dynamic visualization of baselines and their effect using the gWid-gets2 package with GTK+ or Tcl/Tk.

### Usage

```
baselineGUI(spectra, method='irls', labels, rev.x = FALSE)
```

### Arguments

spectra	Matrix with spectra in rows
method	Baseline correction method (optional)
labels	Labels for X-axis (optional)
rev.x	Reverse X-axis (optional, default=FALSE)

### Details

Creates and updates a list containing current baseline and spectrum (baseline.result). Make sure a gWidget2 implementation is available, e.g gWidgets2RGtk2 or gWidgets2tcltk and a corresponding backend like GTK+ or Tcl/Tk. The GUI was developed using GTK which is an external dependency in Windows and OS X.

### Author(s)

Kristian Hovde Liland and Bjørn-Helge Mevik

### Examples

```
data(milk)
## Not run:
# Dependent on external software
baselineGUI(milk$spectra)

## End(Not run)
```

---

custom.baseline	<i>Customized baseline correction</i>
-----------------	---------------------------------------

---

### Description

This function rescales spectrum abscissa by use of breaks and gaps before baseline correction. The effect is that the chosen baseline correction algorithm and parameters will have varying effects along the spectra, effectively giving local control of the amount of rigidity/flexibility of the estimated baseline.

### Usage

```
custom.baseline(spectra, breaks, gaps, trans.win = NULL, just.plot = FALSE, method, ...)
```

### Arguments

spectra	Matrix with spectra in rows.
breaks	Vector of locations of break points between sections of varying baseline flexibility (given as abscissa numbers).
gaps	Vector giving the abscissa spacing between each instance of breaks (and endpoints if not specified in breaks).
trans.win	Optional width of transition window around break points used for smoothing rough breaks by LOWESS (default = NULL).
just.plot	Plot the rescaled spectra instead of applying the customized baseline correction if just.plot=TRUE (default = FALSE).
method	Baseline correction method to use (class character).
...	Additional named arguments to be passed to the baseline correction method.

### Details

This is an implementation of the customized baseline correction suggested by Liland et al. 2011 for local changes in baseline flexibility.

### Value

baseline	Estimated custom baselines.
corrected	Spectra corrected by custom baselines.
spectra.scaled	Re-scaled spectra.
baseline.scaled	Estimated baselines of re-scaled spectra.

### Author(s)

Kristian Hovde Liland and Bjørn-Helge Mevik

## References

Kristian Hovde Liland et al.: Customized baseline correction

## Examples

```
data(milk)
spectrum1 <- milk$spectra[1,1:10000,drop=FALSE]
ordinary <- baseline(spectrum1, method="als", lambda=6, p=0.01)
customized <- custom.baseline(spectrum1, 2900, c(1,20), trans.win=100,
just.plot=FALSE, method="als", lambda=6, p=0.01)
## Not run:
plot(1:10000,spectrum1, type='l')
lines(1:10000,getBaseline(ordinary), lty=2, col=2, lwd=2)
lines(1:10000,customized$baseline, lty=3, col=3, lwd=2)

## End(Not run)
```

---

doOptim

*Optimise several baseline algorithms on a data set*

---

## Description

Tests several baseline algorithms with one predictor for a given data set. The baseline algorithms are represented as a list of [baselineAlgTest](#) objects, and the predictor as a [predictionTest](#) object.

## Usage

```
doOptim(baselineTests, X, y, predictionTest, postproc = NULL,
        tmpfile = "tmp.baseline", verbose = FALSE, cleanTmp = FALSE)
```

## Arguments

baselineTests	a list of <a href="#">baselineAlgTest</a> objects. The baseline algorithms and parameter values to test
X	A matrix. The spectra to use in the test
y	A vector or matrix. The response(s) to use in the test
predictionTest	A <a href="#">predictionTest</a> object. The predictor and parameter values to use in the test
postproc	A function, used to postprocess the baseline corrected spectra prior to prediction testing. The function should take a matrix of spectra as its only argument, and return a matrix of postprocessed spectra
tmpfile	The basename of the files used to store intermediate calculations for checkpointing. Defaults to "tmp.baseline"
verbose	Logical, specifying whether the test should print out progress information. Default is FALSE
cleanTmp	Logical, specifying whether the intermediate files should be deleted when the optimisation has finished. Default is FALSE

**Details**

The function loops through the baseline algorithm tests in `baselineTests`, testing each of them with the given data and prediction test, and collects the results. The results of each baseline algorithm test is saved in a temporary file so that if the optimisation is interrupted, it can be re-run and will use the pre-calculated results. If `cleanTmp` is TRUE, the temporary files are deleted when the whole optimisation has finished.

**Value**

A list with components

<code>baselineTests</code>	The <code>baselineTests</code> argument
<code>results</code>	A list with the <code>baselineAlgResult</code> objects for each baseline test
<code>minQualMeas</code>	The minimum quality measure value
<code>baselineAlg.min</code>	The name of the baseline algorithm giving the minimum quality measure value
<code>param.min</code>	A list with the parameter values corresponding to the minimum quality measure value

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

[baselineAlgTest](#), [predictionTest](#)

---

<code>funcName</code>	<i>Extract the "funcName" slot.</i>
-----------------------	-------------------------------------

---

**Description**

Extract the `funcName` slot from an object of class [baselineAlg](#) or [baselineAlgTest](#)

**Usage**

```
funcName(object)
```

**Arguments**

`object` An object of class [baselineAlg](#) or [baselineAlgTest](#)

**Value**

The `funcName` slot of the object.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

[baselineAlg](#), [baselineAlgTest](#)

---

getBaseline

*Functions to extract the components of a "baseline" object*

---

**Description**

The functions extract the baseline, spectra, corrected or call slot of a [baseline](#) object; usually the result of a call to [baseline](#).

**Usage**

```
getBaseline(object)
getSpectra(object)
getCorrected(object)
getCall(object)
```

**Arguments**

object            A [baseline](#) object

**Value**

getCall returns the baseline call used to create the object. The other functions return a matrix with the original spectra, estimated baselines or corrected spectra.

**Warning**

In a future version, one of the slots might be removed from the class definition and calculated on the fly instead, in order to save space. Therefore, *do* use the extractor functions (getSpectra, getBaseline and getCorrected) instead of accessing the slots directly.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

The function [baseline](#), the class [baseline](#)

**Examples**

```
data(milk)
bl <- baseline(milk$spectra[1:2,])
baseline <- getBaseline(bl)
spectra <- getSpectra(bl)
corrected <- getCorrected(bl)
call <- getCall(bl)
```

---

ind.min

*Extraction methods specific for "predictionResult" objects*

---

**Description**

Extract information from objects of class [predictionResult](#).

**Usage**

```
ind.min(object)
paramName(object)
```

**Arguments**

object            Object of class [predictionResult](#)

**Value**

The corresponding slot of the object.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

[predictionResult](#)

---

milk *MALDI-TOF mass spectra*

---

**Description**

Matrix of 45 spectra of 21451 m/z values from MALDI-TOF on mixed milk samples.

**Usage**

```
data(milk)
```

**Format**

A data frame with 45 observations on the following 2 variables.

cow a numeric vector

spectra a matrix with 21451 columns

**Details**

cow is the concentration of cow milk in mixed samples of cow, goat, and ewe milk.

**References**

Kristian Hovde Liland, Bjørn-Helge Mevik, Elling-Olav Rukke, Trygve Almøy, Morten Skaugen and Tomas Isaksson (2009) Quantitative whole spectrum analysis with MALDI-TOF MS, Part I: Measurement optimisation. *Chemometrics and Intelligent Laboratory Systems*, **96**(2), 210–218.

**Examples**

```
data(milk)
## Not run:
plot(milk$spectra[1,], type = "l")

## End(Not run)
```

---

name *Extraction methods for "baselineAlg" objects*

---

**Description**

Extraction methods specifically for objects of class `baselineAlg`

**Usage**

```
name(object)
description(object)
```



**Arguments**

object            Object of class `baselineAlg`

**Value**

The methods return the corresponding slot of the object.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

`baselineAlg`, `funcName`.

---

optimWizard            *Visual tool for setting up optimization*

---

**Description**

Set up optimization through a graphical user interface. Optionally collecting values directly from 'baselineGUI'. Retrieve optimisation parameters and results with `getOptim` and `getOptimRes`, respectively.

**Usage**

```
optimWizard(X, y, postproc, predictionTest, cvsegments)
getOptim()
getOptimRes()
```

**Arguments**

X                    Matrix with spectra in rows  
y                    Response vector or matrix in analysis  
postproc            Custom function for post processing of spectra (optional)  
predictionTest      Custom prediction object (optional)  
cvsegments          Cross-validation segments (optional)

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

## Examples

```
## Not run:  
# Computationally intensive  
data(milk)  
X <- milk$spectra[,-1]  
y <- milk$spectra[,1]  
optimWizard(X,y)  
  
# After optimisation is complete  
plotOptim(myResults)  
  
## End(Not run)
```

---

overall.min

*Extract the minimum from a baseline optimisation*

---

## Description

Takes the result of an optimisation (a call to [doOptim](#)) and extracts the minimum quality measure value along with the parameters giving rise to the value.

## Usage

```
overall.min(results)
```

## Arguments

results      Result of call to [doOptim](#)

## Value

A list with components

qualMeas      The minimum quality measure value

algorithm      The name of the baseline algorithm corresponding to the minimum

param      A list with the parameter values corresponding to the minimum quality measure value

## Author(s)

Bjørn-Helge Mevik and Kristian Hovde Liland

## See Also

[doOptim](#)

---

param	<i>Extract the "param" slot</i>
-------	---------------------------------

---

**Description**

Extracts the param slot of the object.

**Usage**

```
param(object)
```

**Arguments**

object      An object of class [baselineAlg](#), [baselineAlgTest](#), [baselineAlgResult](#) or [predictionResult](#).

**Value**

The param slot of the object. Usually a data frame, list or numeric.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

Classes [baselineAlg](#), [baselineAlgTest](#), [baselineAlgResult](#), [predictionResult](#)

---

param.ind.min	<i>Extraction methods for "baselineAlgResult" objects</i>
---------------	---

---

**Description**

Extraction methods that are specific for objects of class [baselineAlgResult](#)

**Usage**

```
param.ind.min(object)  
qualMeas.ind.min(object)
```

**Arguments**

object      Object of class [baselineAlgResult](#)

**Value**

The corresponding slot

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

Class [baselineAlgResult](#)

---

plotBaseline *Plot method for "baseline" objects*

---

**Description**

Plot the original spectrum, the estimated baseline, and the corrected spectrum. Optionally zoom and pan plot, either with arguments or interactively.

**Usage**

```
## S4 method for signature 'baseline'
plot(x, y, specNo = 1, grid = FALSE, labels = 1:n, rev.x = FALSE,
     zoom = NULL, ...)
plotBaseline(x, y, specNo = 1, grid = FALSE, labels = 1:n, rev.x = FALSE,
            zoom = list(xz = 1, yz = 1, xc = 0, yc = 0), ...)
```

**Arguments**

x	The baseline object to be plotted
y	Unused. Ignored with a warning
specNo	The row number of the spectrum and baseline to plot. Defaults to 1
grid	Logical. Whether to show a grid or not. Defaults to FALSE
labels	Vector. Labels for the x tick marks. Defaults to 1:n
rev.x	Logical. Whether the spectrum should be reversed. Defaults to FALSE
zoom	Either TRUE (only for the plot method), which turns on the interactive zoom controls, or a list with components xz, xc, yz and yc, which specifies the desired zoom and pan. Defaults to no zoom or pan
...	Other arguments. Currently ignored

**Details**

The normal way to plot baseline objects is to use the plot method. The plotBaseline function is the underlying work-horse function, and is not meant for interactive use.

**Note**

Because the argument list of any plot method must start with x, y, and the plot method for the baseline class does not use the y argument, all arguments except x must be named explicitly. Positional matching will not work.

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

**See Also**

[baseline](#), [baseline](#), [baselineGUI](#)

**Examples**

```
data(milk)
bl <- baseline(milk$spectra[1,, drop=FALSE])
## Not run:
# Computationally intensive
plot(bl)
plot(bl, zoom = TRUE)
## End(Not run)
```

---

plotOptim

*Plotting tool for result objects from optimization*

---

**Description**

A graphical user interface for plotting optimisation results, either one algorithm at the time or comparing algorithms.

**Usage**

```
plotOptim(results)
```

**Arguments**

results      Result list from optimization

**Details**

plotOptim creates a user interface based on the supplied results. Curve and level plots from single algorithms or comparison of algorithms is available.

For single algorithms subsets, levels corresponding to local or global minima, and averages can be extracted for plotting. For comparison of algorithms levels corresponding to local or global minima can be used, or levels corresponding to the minimum when averaging over selected values of the regression parameter, e.g. selected components in PLSR.

**Author(s)**

Kristian Hovde Liland and Bjørn-Helge Mevik

---

PLSRTest-class	Class "PLSRTest"
----------------	------------------

---

### Description

A class describing a PLSR prediction test. To run the test, the "pls" package must be installed.

### Objects from the Class

Objects can be created by calls of the form `new("PLSRTest", ...)`.

### Slots

**ncomp:** Integer vector. The number of PLSR components to test

**cvsegments:** A list of the segments to use in the cross-validation

### Extends

Class [predictionTest](#), directly.

### Methods

**runTest** signature(object = "PLSRTest"): Run the test

### Author(s)

Bjørn-Helge Mevik and Krisitan Hovde Liland

### See Also

The base class [predictionTest](#). The [runTest](#) function. The [pls](#) function from the "pls" package.

### Examples

```
showClass("PLSRTest")
```

---

predictionResult-class  
*Class "predictionResult"*

---

### Description

A class containing the result of running a [predictionTest](#).

### Objects from the Class

The normal way to create objects is by calling the method `runTest` for any object of subclass of [predictionTest](#).

### Slots

**param**: Numeric vector. The regression parameter values tested.  
**qualMeas**: Numeric vector. The quality measure values for each of the values of the `param` slot  
**ind.min**: The index (into `qualMeas`) of the minimum quality measure value  
**minQualMeas**: The minimum quality measure value  
**param.min**: The value of the parameter value corresponding to the minimum quality measure value  
**qualMeasName**: The name of the quality measure  
**paramName**: The name of the regression parameter

### Methods

**ind.min** signature(object = "predictionResult"): Extract the `ind.min` slot  
**minQualMeas** signature(object = "predictionResult"): Extract the `minQualMeas` slot  
**param** signature(object = "predictionResult"): Extract the `param` slot  
**param.min** signature(object = "predictionResult"): Extract the `param.min` slot  
**paramName** signature(object = "predictionResult"): Extract the `paramName` slot  
**qualMeas** signature(object = "predictionResult"): Extract the `qualMeas` slot  
**qualMeasName** signature(object = "predictionResult"): Extract the `qualMeasName` slot

### Author(s)

Bjørn-Helge Mevik and Kristian Hovde Liland

### See Also

Function `runTest`, class [predictionTest](#), subclasses [PLSRTest](#) and [ridgeRegressionTest](#)

### Examples

```
showClass("predictionResult")
```

---

predictionTest-class    *Class "predictionTest"*

---

### Description

A virtual class for all predictor test subclasses. Currently subclasses [PLSRTest](#) and [ridgeRegressionTest](#) are defined.

### Objects from the Class

A virtual Class: No objects may be created from it.

### Methods

No methods defined with class "predictionTest" in the signature.

### Author(s)

Bjørn-Helge Mevik and Kristian Hovde Liland

### See Also

Subclasses [PLSRTest](#) and [ridgeRegressionTest](#).

---

qualMeas                    *Extraction functions for "predictionResult" or "baselineAlgResult" objects*

---

### Description

Extract slots from objects of class [predictionResult](#) or [baselineAlgResult](#).

### Usage

```
qualMeas(object, ...)
## S4 method for signature 'predictionResult'
qualMeas(object, ...)
## S4 method for signature 'baselineAlgResult'
qualMeas(object, ..., MIN, AVG,
  DEFAULT = c("all", "cond.min", "overall.min", "avg"))
minQualMeas(object)
param.min(object)
qualMeasName(object)
```



**Arguments**

object	An object of class <a href="#">predictionResult</a> or <a href="#">baselineAlgResult</a>
MIN	List or vector of parameter names to take the minimum over. Not used if DEFAULT is "cond.min". See Details
AVG	List or vector of parameter names to take the average over. Not used if DEFAULT is "avg". See Details
DEFAULT	Character string. The default way to calculate the minimum (or average) for all parameters. See Details
...	Other arguments. Selection of subsets of parameter levels. See Details

**Details**

The arguments to the [baselineAlgResult](#) method are interpreted in the following way:

Subsets of parameters levels can be selected by supplying their names and specifying the level indices as vectors. Substituting a vector with "all" will return all levels of the corresponding parameter, and substituting it with "overall" will return the level corresponding to the overall minimum. Minimum and average values for selected parameters can be chosen using MIN and AVG, respectively, together with a vector of parameter names.

DEFAULT specifies the action for each remaining parameters: If "all" (default): returns all levels. If "cond.min": take minimum for each remaining parameter (MIN is not used). If "overall.min": set any remaining parameters to their value corresponding to the overall min. If "avg": take average for each remaining parameter (AVG is not used).

**Value**

The qualMeas method for [baselineAlgResult](#) objects returns the subsets or minimum values of the qualMeas slot of the object as specified above. All other methods simply return the corresponding slot.

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

Function [runTest](#), classes [baselineAlgResult](#) and [predictionResult](#)

---

ridgeRegressionTest-class

*Class "ridgeRegressionTest"*

---

**Description**

A class describing a ridge regression test.

**Objects from the Class**

Objects can be created by calls of the form `new("ridgeRegressionTest", ...)`.

**Slots**

`lambda`: Numeric vector. The smoothing parameter values to test

**Extends**

Class `predictionTest`, directly.

**Methods**

**runTest** signature(object = "ridgeRegressionTest"): Run the test

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

The base class `predictionTest`. The `runTest` function.

**Examples**

```
showClass("ridgeRegressionTest")
```

---

runTest	<i>Run a predictionTest or baselineAlgTest</i>
---------	--

---

**Description**

Runs the test defined in a `predictionTest` or `baselineAlgTest` object

**Usage**

```
runTest(object, X, y, ...)
## S4 method for signature 'PLSRTest'
runTest(object, X, y)
## S4 method for signature 'ridgeRegressionTest'
runTest(object, X, y)
## S4 method for signature 'baselineAlgTest'
runTest(object, X, y, predictionTest, postproc, verbose = FALSE)
```

**Arguments**

object	An object of class <code>baselineAlgTest</code> or subclass of <code>predictionTest</code> (currently <code>PLSRTest</code> or <code>ridgeRegressionTest</code> ). The object specify the test to be run
X	A matrix. The spectra to use in the test
y	A vector or matrix. The response(s) to use in the test
predictionTest	A <code>predictionTest</code> object, describing the prediction test to use for this baseline algorithm test
postproc	A function, used to postprocess the baseline corrected spectra prior to prediction testing. The function should take a matrix of spectra as its only argument, and return a matrix of postprocessed spectra
verbose	Logical, specifying whether the test should print out progress information. Default is FALSE
...	Other arguments. Currently only used by the <code>baselineAlgTest</code> method.

**Value**

`runTest` returns an object of class `predictionResult` or `baselineAlgResult`.

**Methods**

`signature(object = "baselineAlgTest")` Baseline corrects the spectra, optionally postprocesses them, and runs a prediction test on the corrected spectra.

`signature(object = "PLSRTest")` Runs PLSR on the data and calculates the cross-validated RMSEP

`signature(object = "ridgeRegressionTest")` Runs ridge regression on the data and calculates the GCV

**Author(s)**

Bjørn-Helge Mevik and Kristian Hovde Liland

**See Also**

`baselineAlgTest`, `predictionTest`, `PLSRTest`, `ridgeRegressionTest`

---

XPSdata

*XPS core line data*

---

**Description**

Matrix of x,y values from X-Ray Photoelectron Spectroscopy on test sample. The data are about the Carbon and Oxygen element for 1s shell.

**Usage**

```
data(C1s)
data(O1s)
```

**Format**

A matrix with the following 2 variables (rows).

first row is the abscissa, ( Binding Energy [eV] )

second row is the Intensity, ( a.u. )

**See Also**

[baseline.shirley](#)

**Examples**

```
data(C1s)
data(O1s)
plot(C1s[1,], C1s[2,], type = "l")
plot(O1s[1,], O1s[2,], type = "l")
```

# Index

- \* **baseline**
  - algorithm, 4
  - baseline, 5
  - baseline-package, 3
  - baseline.als, 7
  - baseline.fillPeaks, 8
  - baseline.irls, 9
  - baseline.lowpass, 10
  - baseline.medianWindow, 11
  - baseline.modpolyfit, 12
  - baseline.peakDetection, 13
  - baseline.rfbaseline, 14
  - baseline.rollingBall, 16
  - baseline.TAP, 19
  - baselineAlgorithms, 22
  - baselineAlgorithmsGUI, 23
  - baselineEnv, 25
  - baselineGUI, 26
  - custom.baseline, 27
  - doOptim, 28
  - funcName, 29
  - getBaseline, 30
  - name, 32
  - optimWizard, 33
  - overall.min, 34
  - param, 35
  - param.ind.min, 35
  - plotBaseline, 36
  - plotOptim, 37
  - qualMeas, 40
  - runTest, 42
- \* **classes**
  - baseline-class, 6
  - baselineAlg-class, 21
  - baselineAlgResult-class, 23
  - baselineAlgTest-class, 24
  - PLSRTest-class, 38
  - predictionResult-class, 39
  - predictionTest-class, 40
  - ridgeRegressionTest-class, 41
- \* **datasets**
  - milk, 32
  - XPSdata, 43
- \* **environment**
  - baselineEnv, 25
- \* **methods**
  - ind.min, 31
  - param, 35
  - qualMeas, 40
  - runTest, 42
- \* **plot**
  - plotBaseline, 36
- \* **spectra**
  - algorithm, 4
  - baseline, 5
  - baseline-package, 3
  - baseline.als, 7
  - baseline.fillPeaks, 8
  - baseline.irls, 9
  - baseline.lowpass, 10
  - baseline.medianWindow, 11
  - baseline.modpolyfit, 12
  - baseline.peakDetection, 13
  - baseline.rfbaseline, 14
  - baseline.rollingBall, 16
  - baseline.TAP, 19
  - baselineGUI, 26
  - custom.baseline, 27
  - doOptim, 28
  - funcName, 29
  - getBaseline, 30
  - name, 32
  - optimWizard, 33
  - overall.min, 34
  - param, 35
  - param.ind.min, 35
  - plotOptim, 37
  - qualMeas, 40

- runTest, 42
- algorithm, 4
- algorithm,baselineAlgTest-method (algorithm), 4
- algorithm-methods (algorithm), 4
- als (baseline.als), 7
- baseline, 5, 5, 6, 7, 19, 30, 37
- baseline-class, 6
- baseline-package, 3
- baseline.als, 5, 7, 26
- baseline.fillPeaks, 5, 8, 26
- baseline.irls, 5, 9, 26
- baseline.lowpass, 5, 10, 26
- baseline.medianWindow, 5, 11, 26
- baseline.modpolyfit, 5, 12, 26
- baseline.peakDetection, 5, 13, 26
- baseline.rfbaseline, 5, 14, 26
- baseline.rollingBall, 5, 16, 26
- baseline.shirley, 5, 17, 44
- baseline.TAP, 5, 19
- baselineAlg, 22, 25, 29, 30, 32, 33, 35
- baselineAlg-class, 21
- baselineAlgorithms, 22
- baselineAlgorithmsGUI, 23
- baselineAlgResult, 25, 35, 36, 40, 41, 43
- baselineAlgResult-class, 23
- baselineAlgTest, 4, 5, 23, 24, 28–30, 35, 42, 43
- baselineAlgTest-class, 24
- baselineEnv, 25
- baselineGUI, 26, 37
- C1s (XPSdata), 43
- custom.baseline, 27
- description (name), 32
- description,baselineAlg-method (name), 32
- description-methods (name), 32
- doOptim, 28, 34
- extraArgs (algorithm), 4
- extraArgs,baselineAlgTest-method (algorithm), 4
- extraArgs-methods (algorithm), 4
- fillPeaks (baseline.fillPeaks), 8
- funcName, 29, 33
- funcName,baselineAlg-method (funcName), 29
- funcName,baselineAlgTest-method (funcName), 29
- funcName-methods (funcName), 29
- getBaseline, 7, 30
- getBaseline,baseline-method (baseline-class), 6
- getBaselineEnv (baselineEnv), 25
- getCall, 7
- getCall (getBaseline), 30
- getCall,baseline-method (baseline-class), 6
- getCorrected, 7
- getCorrected (getBaseline), 30
- getCorrected,baseline-method (baseline-class), 6
- getOptim (optimWizard), 33
- getOptimRes (optimWizard), 33
- getSpectra, 7
- getSpectra (getBaseline), 30
- getSpectra,baseline-method (baseline-class), 6
- ind.min, 31
- ind.min,predictionResult-method (ind.min), 31
- ind.min-methods (ind.min), 31
- irls (baseline.irls), 9
- lowpass (baseline.lowpass), 10
- medianWindow (baseline.medianWindow), 11
- milk, 32
- minQualMeas (qualMeas), 40
- minQualMeas,baselineAlgResult-method (qualMeas), 40
- minQualMeas,predictionResult-method (qualMeas), 40
- minQualMeas-methods (qualMeas), 40
- modpolyfit (baseline.modpolyfit), 12
- mvrValstats (doOptim), 28
- name, 32
- name,baselineAlg-method (name), 32
- name-methods (name), 32
- O1s (XPSdata), 43
- optimWizard, 33

overall.min, 34

param, 35

param,baselineAlg-method (param), 35

param,baselineAlgResult-method (param), 35

param,baselineAlgTest-method (param), 35

param,predictionResult-method (param), 35

param-methods (param), 35

param.ind.min, 35

param.ind.min,baselineAlgResult-method (param.ind.min), 35

param.ind.min-methods (param.ind.min), 35

param.min (qualMeas), 40

param.min,baselineAlgResult-method (qualMeas), 40

param.min,predictionResult-method (qualMeas), 40

param.min-methods (qualMeas), 40

paramName (ind.min), 31

paramName,predictionResult-method (ind.min), 31

paramName-methods (ind.min), 31

peakDetection (baseline.peakDetection), 13

plot,baseline-method (plotBaseline), 36

plotBaseline, 36

plotOptim, 37

plsr, 38

PLSRTest, 39, 40, 43

PLSRTest-class, 38

predictionResult, 31, 35, 40, 41, 43

predictionResult-class, 39

predictionTest, 28, 29, 38, 39, 42, 43

predictionTest-class, 40

putBaselineEnv (baselineEnv), 25

qualMeas, 40

qualMeas,baselineAlgResult-method (qualMeas), 40

qualMeas,predictionResult-method (qualMeas), 40

qualMeas-methods (qualMeas), 40

qualMeas.ind.min (param.ind.min), 35

qualMeas.ind.min,baselineAlgResult-method (param.ind.min), 35

qualMeas.ind.min-methods (param.ind.min), 35

qualMeasName (qualMeas), 40

qualMeasName,baselineAlgResult-method (qualMeas), 40

qualMeasName,predictionResult-method (qualMeas), 40

qualMeasName-methods (qualMeas), 40

rfsbaseline (baseline.rfsbaseline), 14

ridgeRegressionTest, 39, 40, 43

ridgeRegressionTest-class, 41

rollingBall (baseline.rollingBall), 16

runTest, 38, 39, 41, 42, 42

runTest,baselineAlgTest-method (runTest), 42

runTest,PLSRTest-method (runTest), 42

runTest,ridgeRegressionTest-method (runTest), 42

runTest-methods (runTest), 42

shirley (baseline.shirley), 17

TAP (baseline.TAP), 19

XPSdata, 43