Package 'TIMP'

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Type Package

Title a problem solving environment for fitting separable nonlinear models in physics and chemistry applications

Version 1.6

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Depends R (>= 2.7.0), methods, tcltk, vcd, fields, gplots, splines, gclus, nnls (>= 1.1), quadprog, minpack.lm (>= 1.0-9)

Description TIMP is a problem solving environment for fitting separable nonlinear models to measurements arising in physics and chemistry experiments, and has been extensively applied to time-resolved spectroscopy and FLIM-FRET data.

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URL http://timp.r-forge.r-project.org/, http://www.nat.vu.nl/~kate/TIMP/

R topics documented:

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amp-class   *Class "amp" for diagonal matrix model specification.*

Description

amp is the class for diagonal matrix model specification; such models are internally initialized
when a tri-linear-type model is fit to the data via passing the argument opt to fitModel as an
object of class opt in which the slot trilinear has the value TRUE. All objects of class amp
are sub-classes of class dat; see documentation for dat for a description of these slots.

Details

See kin-class for an example of the initialization of a kin object via the initModel function.

Objects from the Class

Objects can be created by calls of the form new("amp", ...) or amp(...).

Slots

amp list of vectors of starting values for the parameters of the amplitudes for each dataset; one
vector of values is used to parameterize the values corresponding to each dataset.

Extends

Class [kin-class](#), directly.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[kin-class](#), [spec-class](#), [opt-class](#)

---

baseIRF	*Baseline subtraction from a vector, usually representing an IRF.*

Description

Baseline subtraction from a vector, usually representing an IRF.

Usage

```
baseIRF(irfvec, indexlow, indexhigh, removeNeg = FALSE)
```

Arguments

irfvec	Vector to subtract a baseline from
indexlow	Lowest index to base the baseline estimation on
indexhigh	Highest index to base the baseline estimation on
removeNeg	Whether negative values should be replaced with 0.

Details

Currently estimates the baseline as the mean of data between indexlow and indexhigh, and subtracts the result from the entire vector.

Value

vector

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

Examples

```
irfvec <- rnorm(128, mean=1)
plot(irfvec,type="l")
irfvec_corrected <- baseIRF(irfvec, 1, 10)
lines(irfvec_corrected, col=2)
```

`dat-class`   *Class "dat" for model and data storage*

Description

`dat` is the super-class of other classes representing models and data, so that other model/data classes (e.g., `kin` and `spec` for kinetic and spectral models respectively) also have the slots defined here. These slots may be specified in the `...` argument of the initModel function.

Objects from the Class

Objects from the class can be created by calls of the form `new("dat", ...)` or `dat(...)`, but most are most often made by invoking another function such as `readData` or `initModel`.

Slots

psi.df: Object of class `"matrix"` dataset from 1 experiment

psi.weight: Object of class `"matrix"` weighted dataset from 1 experiment

x: Object of class `"vector"` time or other independent variable.

nt: Object of class `"integer"` length x

x2: Object of class `"vector"` vector of points in 2nd independent dimension, such as wavelengths of wavenumbers

nl: Object of class `"integer"` length x2

C2: Object of class `"matrix"` concentration matrix for simulated data

E2: Object of class `"matrix"` matrix of spectra for simulated data

sigma: Object of class `"numeric"` noise level in simulated data

mod_type: Object of class `"character"` character string defining the model type, e.g., `"kin"` or `"spec"`

parnames: Object of class `"vector"` vector of parameter names, used internally

finished: Object of class `"logical"` describes whether optimization is complete

simdata: Object of class `"logical"` logical that is `TRUE` if the data is simulated, `FALSE` otherwise; will determine whether values in `C2` and `E2` are plotted with results

weightpar: Object of class `"list"` list of vectors `c(first_x, last_x, first_x2, last_x2, weight)`, where each vector is of length 5 and specifies an interval in which to weight the data.

   first_x first(absolute, not an index) x to weight
   last_x last (absolute, not an index) x to weight
   first_x2 first (absolute, not an index) x2 to weight
   last_x2 last (absolute, not an index) x2 to weight
   weight numeric by which to weight data

Note that if vector elements 1-4 are `NA` (not a number), the firstmost point of the data is taken for elements 1 and 3, and the lastmost points are taken for 2 and 4. For example, `weightpar = list(c(40, 1500, 400, 600, .9), c(NA, NA, 700, 800, .1))` will weight data between times 40 and 1500 picoseconds and 700 and 800 wavelengths by .9, and will weight data at all times between wavelength 700 and 800 by .1. Note also that for single photon counting data `weightpar = list(poisson = TRUE)` will apply poisson weighting to all non-zero elements of the data.

weight: Object of class `"logical"` TRUE when the specification in `weightpar` is to be applied and FALSE otherwise

weightM: Object of class `"matrix"` weights

weightsmooth: Object of class `"list"` type of smoothing to apply with weighting; not currently used

fixed: Object of class `"list"` list of lists or vectors giving the parameter values to fix (at their starting values) during optimization.

free: Object of class `"list"` list of lists or vectors giving the parameter values to free during optimization; if this list is present then all parameters not specified in it are fixed, e.g., `free = list(irfpar = 2)` will fix every parameter at its starting value except for the 2nd `irfpar`. If `fix = list(none=TRUE)` (or if the element `none` has length greater than 0) then all parameters in the model are fixed. Note that this option only should be applied to multiexperiment models in which at least one parameter appling to some other dataset is optimized (`nls` always must have at least one parameter to optimize).

constrained: Object of class `"list"` list whose elements are lists containing a character vector `what`, a vector `ind`, and either (but not both) a character vector `low` and `high`. `what` should specify the parameter type to constrain. `ind` should give the index of the parameter to be constrained, e.g., `1` if indexing into a vector, and `c(1,2)` if indexing into a list. `low` gives a number that the parameter should always remain lower than and `high` gives a number that the parameter should always remain higher than (so that `low` bounds the parameter value from above and `high` bounds the parameter value from below). It is not now possible to specify both `low` and `high` for a single parameter value. An example of a complete `constrained` specification is `constrained = list(list("what = "kinpar", ind = 2, low = .3), list(what = "parmu", ind = c(1,1), high = .002))`

clp0: Object of class `"list"` list of lists with elements `low`, `high` and `comp`, specifying the least value in `x2` to constrain to zero, the greatest value in `x2` to constrain to zero, and the component to which to apply the zero constraint, respectively. e.g., `clp0 = list(list(low=400, high = 600, comp=2), list(low = 600, high = 650, comp=4))` applies zero constraints to the spectra associated with components 2 and 4.

autoclp0: Object of class `"list"` that has two elements; `oldRes`, the output of `fitModel` and an index `ind` representing the index of the dataset to use in `oldRes`; `ind` defaults to one. The clp that are negative in `oldRes` are constrained to zero in the new model; this is primarily useful when fitting a model, finding some negative clp, and constraining them to zero by fitting again with this option. See also the help page for `opt` for other ways to constrain the clp to non-negativity.

makeps: Object of class `"character"` specifyies the prefix of files written to postscript

clpequspec: Object of class `"list"` list of lists each of which has elements `to`, `from`, `low`, `high`, and optional element `dataset` to specify the dataset from which to get the

reference clp (that is, a spectrum for kinetic models). `to` is the component to be fixed in relation to some other component; from is the reference component. `low` and `high` are the least and greatest absolute values of the `clp` vector to constrain. e.g., `clpequspec = list(list(low = 400, high = 600, to = 1, from = 2))` will constrain the first component to equality to the second component between wavelengths 400 and 600. Note that equality constraints are actually constraints to a linear relationship. For each of the equality constraints specfied as a list in the `clpequspec` list, specify a starting value parameterizing this linear relation in the vector `clpequ`; if true equality is desired then fix the corresponding parameter in `clpequ` to 1. Note that if multiple components are constrainted, the from in the sublists should be increasing order, (i.e., `(list(to=2, from=1, low=100, high=10000), list(to=3, from=1, low=10000, high=100))`, not `list(to=3, from=1, low=10000, high=100), list(to=2, from=1, low=10000, high=100))`

lclp0: Object of class `"logical"` TRUE if specification in `clp0` is to be applied and FALSE otherwise

lclpequ: Object of class `"logical"` TRUE if specification in clpequspec is to be applied and FALSE otherwise

title: Object of class `"character"` displayed on output plots

mhist: Object of class `"list"` list describing fitting history

datCall: Object of class `"list"` list of calls to functions

drel vector of starting parameters for dataset scaling relations

dscalspec: Object of class `"list"`

drel: Object of class `"vector"` vector of starting parameters for dataset scaling relations

clpequ: Object of class `"vector"` describes the parameters governing the clp equality constraints specified in `clpequspec`

scalx: Object of class `"numeric"` numeric by which to scale the x axis in plotting

prel vector of starting values for the relations described in prelspec

prel: Object of class `"vector"` vector of starting values for the relations described in prelspec

prelspec: Object of class `"list"` list of lists to specify the functional relationship between parameters, each of which has elements

  what1 character string describing the parameter type to relate, e.g., `"kinpar"`

  what2 the parameter type on which the relation is based; usually the same as `what1`

   ind1 index into `what1`

   ind2 index into `what2`

     rel character string, optional argument to specify functional relation type, by default linear

   e.g., `prelspec = list(list(what1 = "kinpar", what2 = "kinpar", ind1 = 1, ind2 = 5))` relates the 1st element of `kinpar` to the 5th element of `kinpar`. The starting values parameterizing the relationship are given in the `prel` vector

fvecind: Object of class `"vector"` vector containing indices of fixed parameters

pvecind: Object of class `"vector"` used internally to store indices of related parameters.

groups: Object of class `"list"` list containing lists of pairs c(x2 index, dataset index). the `x2` values (which are solved for as conditionally linear parameters) are equated for all pairs in a list.

iter: Object of class `"numeric"` describing the number of iterations that is run; this is sometimes stored after fitting, but has not effect as an argument to `initModel`

clpCon: Object of class `"list"` used internally to enforce constraints on the clp

ncomp: Object of class `"numeric"` describing the number of components in a model

clpdep: Object of class `"logical"` describing whether a model is dependent on the index of x2

inten: Object of class `"matrix"` for use with FLIM data; represents the number of photons per pixel measured over the course of all times t represented by the dataset. See the help for the `readData` function for more information.

positivepar: Object of class `"vector"` containing character strings of those parameter vectors to constrain to positivity, e.g., `positivepar=c("kinpar")`

datafile: Object of class `"character"` containing the name of a datafile associated with the psi.df

clpType: Object of class `"character"` that is "nt" if the model has clp in the "x" dimension and "nl" otherwise (so that, e.g., if `mod_type = "kin"`, then `clpType = "nl"`).

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`kin-class`, `spec-class`

Examples

```
# simulate data

 C <- matrix(nrow = 51, ncol = 2)
 k <- c(.5, 1)
 t <- seq(0, 2, by = 2/50)
 C[, 1] <- exp( - k[1] * t)
 C[, 2] <- exp( - k[2] * t)
 E <- matrix(nrow = 51, ncol = 2)
 wavenum <- seq(18000, 28000, by=200)
 location <- c(25000, 20000)
 delta <- c(5000, 7000)
 amp <- c(1, 2)
 E[, 1] <- amp[1] * exp( - log(2) * (2 * (wavenum - location[1])/delta[1])^2)
 E[, 2] <- amp[2] * exp( - log(2) * (2 * (wavenum - location[2])/delta[2])^2)
 sigma <- .001
 Psi_q  <- C

 # initialize an object of class dat
 Psi_q_data <- dat(psi.df = Psi_q, x = t, nt = length(t),
 x2 = wavenum, nl = length(wavenum))

 # initialize an object of class dat via initModel
 # this dat object is also a kin object
```

```
  kinetic_model <- initModel(mod_type = "kin", seqmod = FALSE,
  kinpar = c(.1, 2))
```

---

divergeZimage	*Plots a matrix with a diverging palette, with the center value of the palettle possible to set*

Description

An image plot of a matrix is a way of visualizing data; when the data represents a quantity like transient absorption, where negative values represent a different phenomena than positive values, it can be useful to set values at zero in the image plot to grey, whereas positive values are assigned to red, and negative values are assigned to blue. Alternately, when comparing image plots of several matrices, it may be useful to set the value assigned to grey uniformly, with values above this threshold assigned to red, and below this threshold assigned to blue.

Usage

```
divergeZimage(ob, out=FALSE, file="divergeZimage.pdf",
                        lin = 1, title = "", center = 0,
                        x2 = vector(), x= vector(),
                        plainmat = FALSE, ylab="wavelength (nm)",
                        xlab = "time (ns)")
```

Arguments

ob	either an object of class dat or a numeric matrix; if a numeric matrix is given then set plainmat=TRUE and specify labels for the columns of matrix in x2 and for the rows of the matrix in x
out	a logical indicating whether to write to the screen in the case that this is possible or to a file; if TRUE, writes to a pdf file
file	a character vector giving a filename to write to in the case that out=TRUE
lin	range of x to plot linearly; values not between $-lin$ and lin are plotted on a log scale
title	character vector giving a title for the plot
center	point assigned to grey in the diverging palette.
x2	vector of labels for the columns of the matrix; used only if plainmat=TRUE
x	vector of labels for the rows of the matrix; used only if plainmat=TRUE
plainmat	logical indicating whether ob is a matrix, as opposed to an object of class dat
ylab	character vector giving a label to put on the y-axis
xlab	character vector giving a label to put on the x-axis

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[dat](#)

| efit2file | *covert 'tim' FORTRAN efit files to plain matrices in ASCII files* |

Description

'tim' efit files sometimes represent spectra associated with multiple datasets; for each matrix of spectra stored in such a file, this function writes a plain text file.

Usage

```
efit2file(filename, skip = 2, numcol, nrows=vector())
```

Arguments

filename	This is the path to the file to read in, as a quoted string.
skip	number of lines at the top of the file before the data begins
numcol	number of columns the data
nrows	a vector saying how many rows are in each of the matrices of spectra in the file; for instance `nrows = c(256,256,256)` would indicate that the file stores spectra associated with 3 datasets, each of which contains 256 wavelengths. If `nrows` is not given, then a single file containing all data is writen.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[readData](#)

---

examineFit   *Examines the results of a call to fitModel*

Description

Examine the results of a call to `fitModel` by a call to plotting functions; call this function with argument an object returned from `fitModel`. Possibly also supply a new specification of plots to be generated.

Usage

```
examineFit(resultfitModel, opt=vector())
```

Arguments

`resultfitModel`
        list returned by a call to `fitModel`

`opt`   possibly an object of class `opt` giving options for plotting; if `opt` has length zero (the default) then the plotting options given in the `opt` list of `resultFitModel` are applied

Details

The `fitModel` function returns a list of results, and initiates plotting functions. Given the `resultfitModel` list `fitModel` returns, `examineFit` initiates the plotting functions, and thus may be used to examine results.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`fitModel`, `opt`

---

fit-class   *Class "fit" to store the results of model fitting associated with all datasets analyzed.*

Description

Class to store results of model fitting associated with all datasets in a single call to the `fitModel` function. An object of class `fit` is stored in the slot `fit` of objects of class `multimodel`.

Objects from the Class

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

Slots

resultlist: Object of class `"list"` that contains an object of class `res` for each dataset modeled, in the order that they were specified.

nlsres: Object of class `"list"` containing named elements

onls output of the call to `nls` used in model optimization.

sumonls result of call `summary(onls)`

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[res-class](), [multimodel-class]()

---

fitModel   *Performs optimization of (possibly multidataset) models.*

Description

Performs optimization of (possibly multidataset) models and outputs plots and files representing the fit of the model to the data.

Usage

```
fitModel(data, modspec=list(), datasetind = vector(), modeldiffs = list(),
              opt = opt() )
```

Arguments

data	list of objects of class `dat` containing the data to be modeled
modspec	list whose elements are models of class `dat` describing the models as results from a call to the function `initModel`
datasetind	vector that has the same length as `data`; for each dataset in `data` specify the model it should have as an index into `modspec`; default mapping is that all datasets use the first model given in `modspec`
modeldiffs	list whose elements specify any dataset-specific model differences.

linkclp list of vectors containing the indices of datasets. If the two dataset indices are in the same vector, their conditionally linear parameters will be equated if they represent the same condition (e.g., a wavelength) within `thresh`. For example, `linkclp = list(1:10, 11:15)` will let datasets 1-10 and 11-15 have the same clp. Note that if `linkclp` is not given, it will default to `list{1:length(data)}`, so that the clp from all datasets are equated when they represent conditions within `thresh` of each other. Consider the situation where the clp from many different datasets are equated. **Then it is important to note that the specification of constraints applicable to the clp will also be equated, and will be read from the model assigned to the first dataset in the group.**

dscal list of lists specifying linear scaling relations between datasets; each list has elements `to, from, value`. The index of the dataset to be scaled is given in `to`; the index of the dataset on which the scaling is to be based is given in `from`. The starting value parameterizing the relationship is given as `value`. For example, `dscal = list(list(to=2,from=1,value=.457))`.

thresh numeric describing the tolerance with which clp from different datasets are to be considered as equal. For instance, for two datasets containing data at 750 and 751 nm, respectively, `thresh=1.5` will equate the clp at 750 and 751 between datasets. Specify a negative value of `thresh` to estimate clp per-dataset. See Section 2.2 of the paper in the references for the model equations.

free list of lists specifying individual parameters to free for a given dataset. each sublist has named elements

what character string naming parameter type, e.g., "kinpar"

ind vector of indices into parameter vector or list, e.g., `c(2,3)` or 4

dataset dataset index in which parameter is to be freed

start starting value for freed parameter

For example, `free = list( list(what = "irfpar", ind = 1, dataset = 2, start=-.1932), list(what = "kinpar", ind = 5, dataset = 2, start=.0004), list(what = "kinpar", ind = 4, dataset = 2, start= .0159))`.

remove list of lists specifying individual parameters to remove from parameter groups for a given dataset. each sublist has named elements

what character string naming parameter type, e.g., "kinpar"

dataset dataset index in which parameter group is to be removed

ind vector of indices into parameter vector or list, e.g., `c(2,3)` or 4 where parameter should be removed

add list of lists specifying individual parameters to add to parameter groups for a given dataset. each sublist has named elements

what character string naming parameter type, e.g., "kinpar"

dataset dataset index in which parameter group is to change

start starting value for added parameter

ind vector of indices into parameter vector or list, e.g., `c(2,3)` or 4 where parameter should be added.

	change	list of lists specifying entire parameter groups to change for a given dataset. each sublist has named elements
	what	character string naming parameter type, e.g., "kinpar"
	dataset	dataset index in which parameter group is to change
	spec	new specification that in initModel would follow "what", e.g., for `c(.1, .3)` if what="kinpar"
	rel	list of lists specifying parameters to relate between datasets each sublist has named elements
	what1	character string naming parameter type to be determined in relation to some other parameter type , e.g., "kinpar"
	what2	character string naming parameter type on which another parameter type is to depend, e.g., "kinpar"
	ind1	vector of indices into parameter vector or list, e.g., `c(2,3)` or `4` of the dependent parameter.
	ind2	vector or numeric of indices into parameter vector or list, e.g., `c(2,3)` or `4` of the parameter on which another parameter will depend
	dataset1	dataset index of the dependent parameter
	dataset2	dataset index of the parameter on which another parameter will depend
	rel	optional character string describing functional relationship between parameters; defaults to "lin" for linear relationship
	start	starting value or vector of values parameterizing relationship between parameters
	weightlist	List of new weights for the datasets returned by the function `outlierCorrs` (as the element `weightList` of the list that is the return value of this function).
opt		Object of class `kinopt` or `specopt` specifying fitting and plotting options.

Details

This function applies the [nls](#) function internally to optimize nonlinear parameters and to solve for conditionally linear parameters (clp) via the partitioned variable projection algorithm.

Value

A list is returned containing the following elements:

currTheta	is a list of objects of class `theta` whose elements contain the parameter estimates associated with each dataset modeled.
currModel	is an object of class `multimodel` containing the results of fitting as well as the model specification
toPlotter	is a list containing all arguments used by the plotting function; it is used to regenerate plots and other output by the `examineFit` function

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Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

References

Mullen KM, van Stokkum IHM (2007). "TIMP: an R package for modeling multi-way spectroscopic measurements." Journal of Statistical Software, 18(3). http://www.jstatsoft.org/v18/i03/.

See Also

readData, initModel, examineFit

FLIMplots   *Functions to plot FLIM results.*

Description

Functions to plot FLIM results.

Usage

```
plotHistAmp(multimodel, t, i=1)
plotHistNormComp(multimodel, t, i=1)
plotIntenImage(multimodel, t, i=1,  tit=c("Intensity Image"))
plotSelIntenImage(multimodel, t, i=1, tit=c("Region of Interest"), cex=1)
plotTau(multimodel, t, i=1, tit=" < tau > ", plotoptions=kinopt())
plotNormComp(multimodel, t, i=1)
```

Arguments

multimodel	the currModel element of the list returned by fitModel
t	the currTheta element of the list returned by fitModel
i	dataset index to make plot for
tit	Character vector giving the title
plotoptions	object of class kinopt giving the plotting options
cex	A numerical value giving the amount by which plotting text and symbols should be magnified relative to the default

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

fitModel

```
getClpindepX-methods
```
Generic function getClpindepX in Package 'TIMP'

Description

Gets the matrix associated with nonlinear parameter estimates for the case that this matrix is not re-calculated per conditionally linear parameter.

Usage

```
getClpindepX(model, multimodel, theta, returnX, rawtheta, dind)
```

Arguments

model	Object of class `dat`; function switches on this argument.
multimodel	Object of class `multimodel` used in standard error determination
theta	Vector of nonlinear parameter estimates.
returnX	logical indicating whether to return a vectorized version of the X matrix
rawtheta	vector of nonlinear parmeters; used in standard error determination
dind	numeric indicating the dataset index; used in standard error determination

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

dat-class

---

getResid	*For data correction, fits a model (but ignores plotting commands) in order to obtain the SVD of the residuals, which then can be used in data-correction.*

Description

For data correction, fits a model exactly as does `fitModel` (but ignores plotting commands) in order to obtain the SVD of the residuals. These residuals can then be subtracted away from the original data to some extent with the `preProcess` function.

Usage

```
getResid(data, modspec=list(), datasetind = vector(), modeldiffs = list(),
                opt = opt() )
```

Arguments

`data`	As in the `fitModel` function
`modspec`	As in the `fitModel` function
`datasetind`	As in the `fitModel` function
`modeldiffs`	As in the `fitModel` function
`opt`	As in the `fitModel` function

Value

list containing the first five left and right singular vectors of the residuals, as well as the first five singular values. A weight matrix (if used) is also included in this list.

See Also

fitModel, preProcess

`getResults`	*Functions to print and return parts of the object returned by the fitting routines.*

Description

Functions to print and return parts of the object returned by `fitModel`. `onls` returns the output of the `nls` function. `sumonls` returns the result of calling `summary` on `onls` function. `parEst` returns a summary of model parameter estimates. The remaining functions return lists representing various aspects of the results returned by the function fitModel.

Usage

```
onls(result)
sumnls(result)
parEst(result, param = "", dataset = NA, verbose = TRUE, file="")
getXList(result, group = vector())
getCLPList(result, getclperr = FALSE)
getData(result, dataset = 1, weighted = FALSE)
getResiduals(result, dataset = 1)
getSVDResiduals(result, numsing = 2, dataset = 1)
getTraces(result, dataset = 1)
getdim1List(result)
getdim2List(result)
```

Arguments

`result`	return value of `fitModel`
`param`	character vector of the particular parameters to return; if `param==""` then all parameters are given.
`dataset`	index of the dataset from which to return results; by default `dataset=NA` in which case results from all datasets are returned
`verbose`	logical that defaults to `TRUE` that determines whether `parEst` just returns a list invisibly or prints as well.
`getclperr`	logical that defaults to `FALSE` that determines whether a list containing the standard error estimates associated with the conditionally linear parameters, as opposed to the conditionally linear parameters themselves
`numsing`	integer that defaults to 2; determines the number of singular vectors to return
`weighted`	logical indicating whether to return weighted or unweighted data
`file`	character vector; if not `""` writes the results to a file with name `file`.
`group`	The value at which to determine the X matrix (maybe a wavelenth index, for example)

Value

`sumnls` returns an object of class `"summary.nls"`.

`onls` returns an object of class `"nls"`.

`parEst` returns an object of class `"list"` representing the parameter estimates.

`XList` returns a `"list"` of length equal to the number of datasets modeled, where each element represents the matrix determined by the nonlinear parameters (under a kinetic model, the concentrations).

`CLPList` returns a `"list"` of length equal to the number of datasets modeled, where each element represents the matrix determined as conditionally linear parameters (under a kinetic model, the spectra).

`getSVDData` returns a `"list"` of length 3 with named elements `values`, `left` and `right`, where `values` contains the singular values, `left` contains `numsing` left singular vectors, and `right` contains `numsing` right singular vectors, all of the unweighted data. The number of singular vectors returned is determined by `numsing`.

`getData` returns the dataset specified by the argument `dataset` (weighted data in the case that `weighted=TRUE`) as a `"matrix"`

`getResiduals` returns a `"matrix"` of residuals for the dataset with index given by the argument `dataset`; the matrix returned has the dimension of the dataset itself.

`getSVDResiduals` returns a `"list"` of length 3 with named elements `values`, `left` and `right`, where `values` contains the singular values, `left` contains `numsing` left singular vectors, and `right` contains `numsing` right singular vectors, all of the residuals. The number of singular vectors returned is determined by `numsing`.

`getTraces` returns a `"matrix"` of model estimates for the dataset with index given by the argument `dataset`; the matrix returned has the dimension of the dataset itself.

getdim1List returns a "list" of length equal to the number of datasets modeled, where each element is a "vector" of length equal to the number of x values in the dataset (times for kinetic models).

getdim2List returns a "list" of length equal to the number of datasets modeled, where each element is a "vector" of length equal to the number of x2 values in the dataset (wavelengths for kinetic models).

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

fitModel

---

initModel	*Defines the model to be used in analysis.*

Description

Allows definition of a model of class "dat" to be used in analysis. The arguments specify the model.

Usage

```
initModel(...)
```

Arguments

...   specify the model class via the character string e.g., kin-class or spec and any of the slots associated with that model type (which is a subclass of class dat, so that all slots in dat may also be specified), e.g., mod_type = "kin" will initialize a model with class kin, for a kinetic model.

Details

For examples, see the help files for dat-class and fitModel

Value

an object of class dat with the sub-class given by the value of the mod_type input.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

dat-class, kin-class, spec-class, fitModel

`Internals`	*TIMP function used internally*

Description

TIMP function used internally

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

baseIRF, readData, preProcess, initModel, fitModel, examineFit, sumKinSpecEst

---

`kin-class`	*Class "kin" for kinetic model storage.*

Description

`kin` is the class for kinetic models; an object of class "kin" is initialized if `mod_type = "kin"` is an argument of `initModel`. All objects of class `kin` are sub-classes of class `dat`; see documentation for `dat` for a description of these slots.

Details

See dat-class for an example of the initialization of a `kin` object via the `initModel` function.

Objects from the Class

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

Slots

kinpar vector of rate constants to be used as starting values for the exponential decay of components; the length of this vector determines the number of components of the kinetic model.

specpar: Object of class `"list"` parameters for spectral constraints

seqmod: Object of class `"logical"` that is TRUE if a sequential model is to be applied and FALSE otherwise

irf: Object of class `"logical"` that is TRUE is an IRF is modeled and FALSE otherwise

mirf: Object of class `"logical"` that is TRUE if a measured IRF is modeled and FALSE otherwise

measured_irf: Object of class `"vector"` containing a measured IRF

convalg: Object of class "numeric" 1-3 determining the numerical convolution algorithm used in
    the case of modeling a measured IRF; if 3 then supply a reference lifetime in the slot reftau.

reftau: Object of class "numeric" containing a reference lifetime to be used when convalg=3

irffun: Object of class "character" describing the function to use to describe the IRF, by default
    "gaus"

irfpar: Object of class "vector" of IRF parameters; for the common Gaussian IRF this vector is
    ordered c(location, width)

dispmu: Object of class "logical" that is TRUE if dispersion of the parameter for IRF location is to
    be modeled and FALSE otherwise

dispmufun: Object of class "character" describing the functional form of the dispersion of the
    IRF location parameter; if equal to "discrete" then the IRF location is shifted per element of x2 and
    parmu should have the same length as x2. defaults to a polynomial description

parmu: Object of class "list" of starting values for the dispersion model for the IRF location

disptau: Object of class "logical" that is TRUE if dispersion of the parameter for IRF width is to
    be modeled and FALSE otherwise

disptaufun: Object of class "character" describing the functional form of the dispersion of the
    IRF width parameter; if equal to "discrete" then the IRF width is parameterized per element of
    x2 and partau should have the same length as x2. defaults to a polynomial description

partau: Object of class "vector" of starting values for the dispersion model for the IRF FWHM

fullk: Object of class "logical" that is TRUE if the data are to be modeled using a compartmental
    model defined in a K matrix and FALSE otherwise

kmat: Object of class "array" containing the K matrix descriptive of a compartmental model

jvec: Object of class "vector" containing the J vector descriptive of the inputs to a compartmental
    model

ncolc: Object of class "vector" describing the number of columns of the C matrix for each clp in x2

kinscal: Object of class "vector" of starting values for branching parameters in a compartmental
    model

kmatfit: Object of class "array" of fitted values for a compartmental model

cohspec: Object of class "list" describing the model for coherent artifact/scatter component(s) con-
    taining the element type and optionally the element numdatasets. The element type can be
    set as follows:

    "irf": if type="irf", the coherent artifact/scatter has the time profile of the IRF.

    "freeirfdisp": if type="freeirfdisp", the coherent artifact/scatter has a Gaussian time
        profile whose location and width are parameterized in the vector coh.

    "irfmulti": if type="irfmulti" the time profile of the IRF is used for the coherent arti-
        fact/scatter model, but the IRF parameters are taken per dataset (for the multidataset case),
        and the integer argument numdatasets must be equal to the number of datasets modeled.

"seq": if type="seq" a sequential exponential decay model is applied, whose starting value are contained in an additional list element start. This often models oscillating behavior well, where the number of oscillations is the number of parameter starting values given in start. The starting values after optimization will be found in the slot coh of the object of class theta corresponding to each dataset modeled.

"mix": if type="mix" if type="mix" a sequential exponential decay model is applied along with a model that follows the time profile of the IRF; the coherent artifact/scatter is then a linear superposition of these two models; see the above description of seq for how to supply the starting values.

coh: Object of class "vector" of starting values for the parameterization of a coherent artifact

wavedep: Object of class "logical" describing whether the kinetic model is dependent on x2 index (i.e., whether there is clp-dependence)

lambdac: Object of class "numeric" for the center wavelength to be used in a polynomial description of x2-dependence

amplitudes: Object of class "vector" that may be used to multiply the concentrations by a square diagonal matrix with the number of columns that the concentration matrix has; the diagonal is given in amplitudes and these values will be treated as parameters to be optimized.

streak: Object of class "logical" that defaults to FALSE; if streak=TRUE then the period of the laser is expected via streakT.

streakT: Object of class "numeric" the period of the laser; this will be used to add a backsweep term to the concentration matrix and should be set in conjunction streak=TRUE.

doublegaus: Object of class "logical" that defaults to FALSE and determines whether a double Gaussian should be used to model the IRF. If doublegaus=TRUE then irfpar should contain four numeric values corresponding to the location (mean) of the IRF, the FWHM of the first Gaussian, the FWHM of the second Gaussian, and the relative amplitude of the second Gaussian, respectively.

Extends

Class dat-class, directly.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

dat-class, spec-class

---

kinopt-class   *Class "kinopt" stores options for fitting and plotting kinetic models*

Description

Class "kinopt" stores options for fitting and plotting kinetic models in particular; this is a subclass of class `opt`

Details

See `opt-class` for the specification of fitting/plotting options that are not specific to the class type.

Objects from the Class

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

Slots

notraces: Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, do not plot traces

selectedtraces: Object of class `"vector"` containing x indices for which plots of traces are desired under a kinetic model

breakdown: Object of class `"list"` with the following elements:

    plot vector of x2 values to plot the breakdown for. These values be specified in a fuzzy way: an x2 value within `abs(x2[1] - x2[2])/100` a value given in `plot` means that a plot for that x2 value will be generated, where the reference `x2[1]` and `x2[2]` are from the first dataset modelled.

    tol numeric giving a tolerance by which the values in `plot` are compared to x2 values for near-equality. The default is defined as `abs(x2[1] - x2[2])/100`.

superimpose vector of dataset indices for which results should be superimposed if the dataset has an x2 value at a value in `plot`.

FLIM: Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, the data represent a FLIM experiment and special plots are generated.

FLIMresidimag: Object of class `"logical"` that defaults to `TRUE`; if `FALSE` and a FLIM image is analyzed, the residuals are not plotted as an image.

noFLIMsummary: Object of class `"logical"` that defaults to `FALSE`; if `TRUE` and a FLIM image is analyzed, only other plots requested by the user (such as traces or residuals) are generated, and no summary plot in made.

kinspecest Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, make a plot of the spectra associated with the kinetic components as well as the lifetime estimates.

writeplaincon Object of class `"list"`; if length is greater than 0, then the concentration model will be evaluated at the vector of x values supplied as the element `"x"` of `writeplaincon` and the result will be written to file for each dataset.

writerawcon Object of class `"logical"` that defaults to FALSE; if TRUE, then the representation of the concentration profiles before the application of constraints (to account for the equality of spectra, etc.) is written to file for each dataset.

plotcohcolspec Object of class `"logical"` that defaults to TRUE; if FALSE then the spectra associated with the coherent artifact (pulse-follower) are not included in the summary plots

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

examineFit, fitModel, opt-class, specopt-class

---

mass-class   *Class "mass" for mass spectrometry model storage.*

Description

`mass` is the class for mass spectrometry models; an object of class "mass" is initialized if `mod_type = "mass"` is an argument of `initModel`. All objects of class `mass` are sub-classes of class `kin`; see documentation for `kin` for a description of these slots.

Details

See kin-class for an example of the initialization of a `kin` object via the `initModel` function.

Objects from the Class

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

Slots

peakpar list of vectors of starting values for the parameters of components; one vector of values is used to parameterize each component.

peakfunct: Object of class `"character"` that specifies the function by which components are parameterized in time; this is by default "expmodgaus" for the exponentially modified Gaussian function.

lzerofile: Object of class `"character"` that specifies the filename of the lzero specification to read in from file. This file has the format: 1st line not read; lines thereafter are the space-delimited index of the component to constrain, the lower bound of the constraint, and the upper bound of the constraint, e.g., `1 218.800000000000011 220.099999999999994`

extracomp: Object of class `"logical"` that defaults to TRUE and determines whether a component with constant concentration in time is added to the model to represent a baseline.

shift: Object of class `"vector"` that represents a shift of the location of each elution profile peak; this can be specified per-component, in which case `length(shift)` is the number of components (not including a baseline component) or for all components, in which case `length(shift == 1)`.

Extends

Class `kin-class`, directly.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`kin-class`, `spec-class`

---

massopt-class	*Class "massopt" stores options for fitting and plotting models for mass spectrometry data*

Description

Class "massopt" stores options for fitting and plotting models models for mass spectrometry data in particular; this is a subclass of class `opt` that contains options applicable to all model types

Details

See `opt-class` and for the specification of fitting/plotting options that are not specific to the `mass` class type.

Objects from the Class

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

Slots

axis.by: Object of class `"numeric"` that allows labels on the bars representing the mass spectra to to skipped, e.g., `axis.by=2` will add a label to every second bar

scale.concen: Object of class `"logical"` that scales the concentration matrix using the algorithm found in the function `scaleConList`.

nummaxtraces: Object of class `"nummaxtraces"` that defaults to zero; if greater than zero then this number of the traces with the maximum amplitude are plotted

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`examineFit`, `fitModel`, `opt-class`, `specopt-class`

---

modifyModel	*Allows the starting values for parameters associated with a model to be updated with the values found in fitting the model.*

Description

Allows the starting values for parameters associated with a model to be updated with the values found in fitting the model. That is, a model is specified with initModel. Then fitModel is used to optimize the starting values for parameters. modifyModel allows modifification of the starting values in the model specification with the optimized values found via fitModel.

Usage

```
modifyModel(model = list(), newest = list(), exceptslots = vector() )
```

Arguments

model	an object of class dat returned by initModel; if this argument is of length(0), which is the default, then the last model fit is used (which is found in the global variable .currModel@model)
newest	an object of class theta containing new parameter estimates; if this argument is of length(0), which is the default, then the parameter estimates associated with dataset 1 in the last model fit are used (which are found in the global variable .currTheta[[1]])
exceptslots	a vector of character vector of slot names whose corresponding slots are to be left out of the update

Value

an object of class dat that returns the results of calling initModel with the new starting values.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

initModel, fitModel

---

multimodel-class   *Class "multimodel" for storage of multidataset models, data and the*
                          results of fitting.

Description

`multimodel` is the class to store data, a generally applicable model, a list of per-data models, a specification of per-dataset model differences, and results for the analysis of possibly many datasets. After a call to `fitModel` an object is initialized of the `multimodel` class.

Details

after a call to `fitModel`, an object of class `multimodel` exists in the global environment as the variable `currModel`

Objects from the Class

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

Slots

data: Object of class `"list"` of objects of class `dat` containing data

model: Object of class `"dat"` of class dat containing a model specification to be applied to all datasets

modellist: Object of class `"list"` of length n where n is the number of datasets given in `data`, and each element i is an object of class `dat` giving the dataset-specific model applicable to `data[[i]]`

modeldiffs: Object of class `"list"` of per-dataset model differences input as an argument to the `fitModel` function

fit: Object of class `"fit"` containing a list of results per-dataset as well as the output of optimization returned by the `nls` function.

groups: Object of class `"list"` containing a list of lists of the groups of clp to link across datasets. Each component list contains vectors of form (clp condition index, dataset index), and such vectors in the same component list are linked between datasets. See `fitModel` for more details on the linking possibilities.

stderrclp: Object of class `"logical"` describing whether standard error estimates on conditionally linear parameters should be calculated; this is determined by the `opt` argument of `fitModel` and defaults to `FALSE`

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`fitModel`

`multitheta-class`	*Class "multitheta" that stores a list with one element of class "theta" for each dataset modeled.*

Description

Class `multitheta` stores a list with one element of class `theta` for each dataset modeled, corresponding to the parameter estimates associated with that dataset.

Objects from the Class

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

Slots

th: Object of class `"list"` with element i corresponding to the `theta` object for the ith dataset modeled.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[theta-class](#), [dat-class](#)

`opt-class`	*Class "opt" stores options for fitting and plotting*

Description

Class "opt" stores options for fitting and plotting applicable to all model types

Details

See [kinopt-class](#), [specopt-class](#) and [massopt-class](#) for the specification of fitting/plotting options that are specific to the class type.

Objects from the Class

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

Slots

> **algorithm:** Object of class `"character"` that defaults to `algorithm="nls"`, so that the
> function `nls` is used to optimize nonlinear parameters under least squares criteria. Other
> options are
>
>> **nls.lm:** optimize nonlinear parameters under least squares criteria using `nls.lm`
>>
>> **optim:** optimize nonlinear parameters under poisson regression criteria with the Nelder-
>> Mead algorithm in `optim`; if this option is used then it MUST be used in conjunction
>> with `nnls=TRUE`. Currently, it must also be used with `stderrclp=FALSE`.
>
> **nnls:** Object of class `"logical"` that defaults to `FALSE`. If `nnls=TRUE`, constrain the condi-
> tionally linear parameters to nonnegativity via a nonnegative least squares algorithm as imple-
> mented via the function `nnls` from the package by the same name.
>
> **writecon:** Object of class `"logical"` that defaults to `FALSE`; if true then concentrations are
> written to a txt file; row labels are `x`
>
> **writespec:** Object of class `"logical"` that defaults to `FALSE`; if `TRUE` then spectra are writ-
> ten to a txt file; row labels are `x2`
>
> **writenormspec:** Object of class `"logical"` that defaults to `FALSE`; if `TRUE` then normalized
> spectra are written to a txt file; row labels are `x2`
>
> **writefit:** Object of class `"logical"` that defaults to `FALSE`; if `TRUE` then fit is written to a
> txt file; row and column labels are `x` and `x2`
>
> **writeclperr:** Object of class `"logical"` that defaults to FALSE; if true then the error bars
> for clp are written to a txt file. This option is only sensible with `stderrclp=TRUE`.
>
> **output:** Object of class `"character"` that defaults to `"ps"`, which means that plots written
> to file are postscript. Alternatively, specify `output = "pdf"`, and plots are written as pdf
> files
>
> **addfilename:** Object of class `"logical"` that, for each data file, tries to add the filename to
> plots associated with output for that data.
>
> **residplot:** Object of class `"logical"` defaults to `FALSE`; if `TRUE` generate a plot of residu-
> als in a separate window.
>
> **plot:** Object of class `"logical"` that defaults to `TRUE`; if `FALSE` then do not write output in
> the form of plots and other windows to the screen.
>
> **divdrel:** Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, plot traces and concen-
> tration profiles divided by the dataset scaling parameters where they apply; this allows for the
> fit of datasets having different intensities on the same scale.
>
> **plotkinspec:** Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, generates a sep-
> arate plot of the spectra associated with the components that are not a part of a coherent
> artifact/scatter model.
>
> **superimpose:** Object of class `"vector"` containing dataset indices whose results should be
> superimposed in plots
>
> **xlab:** Object of class `"character"` containing label for x-axis, e.g., `"nanoseconds"` or
> `"picoseconds"`
>
> **ylab:** Object of class `"character"` containing label for y-axis, e.g., `"wavelength"`
>
> **title:** Object of class `"character"` containing title to write at the top of plots.

makeps: Object of class `"character"` containing prefix to plot files written to postscript; if present postscript will be written. Note that this string is also used as the preffix of txt output files

linrange: Object of class `"numeric"` giving linear range of time axis for plotting; time will be plotted linearly from -linrange to linrange and plotted on a logarithmic (base 10) axis elsewhere

summaryplotrow: Object of class `"numeric"` giving number of rows in summary plot; defaults to 4

summaryplotcol: Object of class `"numeric"` giving number of columns in summary plot; defaults to 4

iter: Object of class `"numeric"` giving number of iterations to optimize model parameters; if `nls=FALSE` so that the Levenberg-Marquardt algorithm is applied, then `iter` is interpretted as the maximum number of residual function evaluations (see the help page of the function `nls.lm` for details)

paropt: Object of class `"list"` of graphical parameters in format `par(...)` to apply to plots.

stderrclp: Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, estimates of the standard error of conditionally linear parameters are made

addest: Object of class `"vector"` containing character strings of which parameter estimates should be added to the summary plot, e.g., `addest = c("kinpar", "irfpar")`

kinspecerr Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, add standard error estimates to the clp a plot generated with `kinspecest=TRUE` or `plotkinspec=TRUE`. This option can only be used if the estimates were generated during fitting via the option `stderrclp=TRUE`

xlimspec Object of class `"vector"` that defaults to `vector()`; if changed, it should specify the desired x-limits of the plot of clp

ylimspec Object of class `"vector"` that defaults to `vector()`; if changed, it should specify the desired y-limits of the plot of clp. In the case of plotting the results of FLIM image analysis, `ylimspec` can be used to determine the range used in the image plot of lifetimes.

ylimspecplus Object of class `"vector"` that defaults to `vector()`; if changed, the first value should specify a vector to add to the y-limits of the plot of clp

samespecline Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, then the line-type for clp is the same for all datasets

specinterpol Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, use spline instead of lines between the points representing estimated clp

specinterpolpoints Object of class `"logical"` that defaults to `TRUE`; if `TRUE`, add points representing the actual estimates for clp to plots of the curves respresenting smoothed clp

specinterpolseg Object of class `"numeric"` that defaults to `50`; represents the number of segments used in a spline-based representation of clp

specinterpolbspline Object of class `"logical"` that defaults to `FALSE`; determines whether a B-spline based representation of clp is used (when `specinterpol=TRUE`) or a piecewise polynomial representation

normspec Object of class `"logical"` that determines whether clp are normalized in plots

writespecinterpol Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, a spline-based representation of clp is written to ASCII files

nlsalgorithm Object of class `"character"` that defaults to `"default"` and determines the algorithm used by `nls`, if `nls` is used in optimization. See `help(nls)` for other possibilities, such as `"port"`, which is more stable with respect to starting values but requires more time.

ltyfit Object of class `"numeric"` if given, sets the line type of the fit in plots of the fit/data; see `lty` in `help(par)` for options.

ltydata Object of class `"numeric"` if given, sets the line type of the data in plots of the fit/data; see `lty` in `help(par)` for options.

colfit Object of class `"vector"` if given, sets the color of the fit corresponding to each dataset in plots of the fit/data; see `col` in `help(par)` for options. If given `length(colfit)` must be equal to the number of datasets in the analysis

coldata Object of class `"vector"` if given, sets the color of the data for each dataset in plots of the fit/data; see `col` in `help(par)` for options. If given, `length(coldata)` must be equal to the number of datasets in the analysis

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[kinopt-class](), [specopt-class]()

---

outlierCorr	*Finds and removes outliers from a datasets*

Description

Finds and removes outliers from datasets given the results of fitting as returned by `fitModel`. Uses the residuals in the fitted results to return a list of corrected datasets to be used in place of the datasets used in the call to `fitModel` as well as a list of weights. The data returned contains the fitted values at pointed that are outliers and will be assigned zero weight in subsequent fits.

Usage

```
outlierCorr(oldRes, fence=3, saturCorr=FALSE, saturThresh=.05,
                        saturMin=NA, saturDivMax=3, outlierCorr=TRUE,
                        newM = TRUE)
```

Arguments

`oldRes`	Object returned by `fitModel` function
`fence`	Object of class `"numeric"` determining what points to consider outliers.
`saturCorr`	whether to correct for saturation
`saturThresh`	See code.
`saturMin`	See code.

`saturDivMax`	See code.
`outlierCorr`	whether to perform outlier correction
`newM`	whether to add to the outliers and saturation points detected previousely

Details

We calculate the fourth spread at a given value of `x2` in a dataset. Those points that are less than the first quartile minus the fourth spread times `fence` are outliers, as are those points that are more than the third quartile plus the fourth spread times `fence`. Outliers are assigned a weight of zero and are assigned the values found in fitting for the purpose of generating smooth-looking plots.

Value

list containing the elements `dt`, a list of corrected datasets, and `weightList`, a list of new weight matrices.

See Also

`fitModel, preProcess`

---

plotter-methods	*Generic function plotter in Package 'TIMP'*

Description

Methods for function `plotter` in Package 'TIMP' that call plotting and output functions.

Usage

```
plotter(model, multimodel, multitheta, plotoptions)
```

Arguments

`model`	Object of class `dat`; function switches on this argument.
`multimodel`	Object of class `multimodel`
`multitheta`	Object of class `multitheta`
`plotoptions`	list of output options input to `fitModel` as the argument `opt`

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`dat-class`

---

preProcess   *Performs preprocessing on data stored as an objects of class dat.*

Description

Performs data sampling, selection, baseline correction, scaling, and data correction on an object of class dat.

Usage

```
preProcess(data, sample = 1, sample_time = 1, sample_lambda = 1,
    sel_time = vector(), sel_lambda = vector(), baselinetime = vector(),
    baselinelambda = vector(), scalx = NULL, scalx2 = NULL,
    sel_lambda_ab = vector(), sel_time_ab = vector(), rm_x2=vector(),
    rm_x = vector(), svdResid = list(), numV = 0, sel_special = list())
```

Arguments

data	Object of class dat
sample	integer describing sampling interval to take in both time and x2; e.g., sample=2 will sample every 2nd time and every 2nd point in x2.
sample_time	integer describing sampling interval in time; e.g., sample_time=2 will sample every 2nd element of the time vector.
sample_lambda	
	integer describing sampling interval in x2; e.g., sample_lambda=2 will sample every 2nd element in the x2 vector.
sel_time	vector of length 2 describing the first and last time index of data to select; e.g., sel_time=c(5,120) will select data at times indexed 5-120.
sel_lambda	vector of length 2 describing the first and last x2 index of data to select; e.g., sel_lambda=c(5,120) will select data at x2 indexed 5-120.
baselinetime	a vector of form c(timeIndexmin, timeIndexmax, lambdaIndexmin, lambdaIndexmax). The average of data between x2 indexes lambdaIndexmin and lambdaIndexmax is subtracted from data with time index between timeIndexmin and timeIndexmax.
baselinelambda	
	a vector of form c(timeIndexmin, timeIndexmax, lambdaIndexmin, lambdaIndexmax). The average of data between time indexes timeIndexmin and timeIndexmax is subtracted from data with x2 index between lambdaIndexmin and lambdaIndexmax.
scalx	numeric by which to linearly scale the x axis (which often represents time), so that newx = oldx * scalx
scalx2	vector of length 2 by which to linearly scale the x2 axis, so that newx2 = oldx2 * scalx2[1] + scalx2[2]

sel_lambda_ab

> vector of length 2 describing the absolute values (e.g., wavelengths, wavenumbers, etc.) between which data should be selected. e.g., `sel_lambda_ab = c(400, 600)` will select data associated with `x2` values between 400 and 600.

sel_time_ab   vector of length 2 describing the absolute times between which data should be selected. e.g., `sel_time_ab = c(50, 5000)` will select data associated with time values between 50 and 5000 picoseconds.

rm_x2   vector of `x2` indices to remove from the data

rm_x   vector of `x` indices to remove from the data

svdResid   list returned from the `getResid` function, containing residuals to be used in data correction.

numV   numeric specifying how many singular vectors to use in data correction. Maximum is five.

sel_special   list of lists specifying `x` indices to remove from individual wavelength ranges, e.g., `sel_special = list(c(400,600,10,12),c(600,800,11,13))` indicates that between wavelength 400 and 600, time indices between 10 and 12 should be removed from the data, and between wavelengths 600 and 800, time indices between 11 and 13 should be removed from the data. Note that the number of time indices to remove should be the same in each wavelength interval specified. Also note that the time vector associated with the data after the first set of indices is removed will be associated with the resulting dataset.

Value

object of class `dat`.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[readData](#), [getResid](#)

---

readclp0	*This function reads in a specification of constraints to zero on the clp.*

Description

This function is useful for the case that there are many constraints to zero in the model, as is the case for some mass spectrometry models.

Usage

```
readclp0(filenm)
```

Arguments

filenm   Object of class `"character"` that gives is the path to the file to read in.

Details

The file to be read in should have the following format: 1st line is not read. Lines thereafter are the space-delimited index of the component to constrain, the lower bound of the constraint, and the upper bound of the constraint, e.g., `1 218.800000000000011 220.099999999999994`.

Value

The constraints to zero in the format documented in the help file for the `"dat"` class. Therefore a call to `"readclp0"` may be used inside a call to `"initModel"`, as in `clp0 = readclp0("filename")`.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[initModel](#)

---

readData	*This function reads in data the ivo file format*

Description

Data in the formats described at <http://www.nat.vu.nl/~kate/TIM/tim/node74.html> and <http://www.nat.vu.nl/~kate/FLIM_format> may be read from file into an R object for analysis.

Usage

```
readData(filenm, typ="", sep = "")
```

Arguments

filenm   This is the path to the file to read in, as a quoted string.

typ   if `typ="plain"` the the file being read in stores data as a plain matrix, with `x` values as the first element of each row except the first and `x2` values as the first row.

sep   This is an optional argument describing how the data is delimited; defaults to `""`

Value

an object of class `dat`

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[preProcess](#)

---

res-class	*Class "res" to store the results of model fitting associated with a single dataset.*

Description

Class to store results of model fitting associated with a single dataset. A list containing objects of class res is a slot in class fit. An object of class fit is stored in the slot fit of objects of class multimodel.

Objects from the Class

Objects can be created by calls of the form new("res", ...). A res object is created after model fitting via the residual function residPart.

Slots

cp: Object of class "list" that contains the estimates for conditionally linear parameters.

resid: Object of class "list" of residuals, with one element for each dataset modeled.

fitted: Object of class "list" of fits, with one element for each dataset modeled.

irfvec: Object of class "list" with a vector of elements for each element of the clp x2

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

[fit-class](#), [multimodel-class](#)

residPart-methods   *Generic function residPart in Package 'TIMP'*

Description

Methods for function `residPart` in Package 'TIMP' determine the part of the residual vector
associated with a single 'part' of the dataset(s).

Usage

```
residPart(model, group, multimodel, thetalist, clpindepX, finished, returnX,
rawtheta)
```

Arguments

`model`	Object of class `dat`; switches on this argument.
`group`	list of vector pairs (x2 index, dataset index) for which the part of the residual vector is to be determined
`multimodel`	Object of class `multimodel`
`thetalist`	Object of class `multitheta`
`clpindepX`	Object of class `matrix` containing the matrix determined directly by the nonlinear parameters (e.g., a concentration matrix in the case of a kinetic model) in the case that this matrix does not depend on the `x2` index
`finished`	logical determining whether fitting is finished that triggers the storage of results
`returnX`	logical determining whether to just return the matrix `X` directly dependent on nonlinear parameters; this is used in the finite difference derivative of `X` used to get standard error estimates on the conditionally linear parameters.
`rawtheta`	numeric vector of nonlinear parameters to be optimized by `nls`; this is used in the finite difference derivative of `X` used to get standard error estimates on the conditionally linear parameters.

See Also

dat-class, spec-class, kin-class

---

spec-class   *Class "spec" for the storage of spectral models.*

Description

spec is the class for spectral models; an object of class "mass" is initialized if mod_type = "spec" is an argument of initModel. All objects of class spec are also of class dat; see documentation for dat for a description of these slots. Note that here x2 will refer to the independent variable in which traces are resolved, e.g., wavelength or wavenumber.

Objects from the Class

Objects can be created by calls of the form new("spec", ...) or spec(...).

Slots

clpequ: Object of class "vector" of starting values for linear relationships between clp

specpar: Object of class "list" of vectors of starting values for spectral parameters; the number of vectors gives the number of components in the resulting spectral model; each vector contains the parameters associated with a component. e.g., specpar = list(c(20000, 3000, .3, 21000, 2000, .4), c(18000, 1000, .2)); the parameters in each vector are grouped c(location_spectra, width_spectra, skew_spectra). the location and width parameters are given in wavenumbers.

specfun: Object of class "character", "gaus" for a spectral model of a superposition of skewed Gaussians; "bspline" for a bspline-based model.

specref: Object of class "numeric" index defining the center value of the x2 variable.

specCon: Object of class "list" used internally to store constraints.

specdisp: Object of class "logical" TRUE if time-dependence of the spectral parameters is to be taken into account and FALSE otherwise

specdisppar: Object of class "list"

specdispindex: Object of class "list" of vectors defining those indexes of specpar whose time-dependence is to be modeled. e.g., specdispindex = list(c(1,1), c(1,2), c(1,3)) says that parameters 1-3 of spectra 1 are to be modeled as time-dependent.

nupow: Object of class "numeric" describing the power to which wavenumbers are raised in the model equation; see Equation 30 of the paper in the references section for a complete description

timedep: Object of class "logical" describing whether the model for spectra E is dependent on x-index (i.e., whether it is clp-dependent).

parmufunc: Object of class "character" describing the function form of the time-dependence of spectral parameters; options are "exp" for exponential time dependence, "multiexp" for multiexponential time dependence, and "poly" for polynomial time dependence. defaults to polynomial time dependence.

ncole vector describing the number of columns of the E matrix for each value in the x vector

Extends

Class `dat-class`, directly.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

References

Ivo H. M. van Stokkum, "Global and target analysis of time-resolved spectra, Lecture notes for the Troisieme Cycle de la Physique en Suisse Romande", Department of Physics and Astronomy, Faculty of Sciences, Vrije Universiteit, Amsterdam, The Netherlands, 2005, `http://www.nat.vu.nl/~ivo/lecturenotes.pdf`

See Also

`kin-class`, `dat-class`

---

specopt-class	*Class "specopt" stores options for fitting and plotting spectral models*

Description

Class "specopt" stores options for fitting and plotting spectral models in particular; this is a subclass of class `opt`.

Details

See `opt-class` for the specification of fitting/plotting options that are not specific to the class type.

Objects from the Class

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

Slots

nospectra: Object of class `"logical"` that defaults to `FALSE`; if `TRUE`, do not plot time-resolved spectra

selectedspectra: Object of class `"vector"` containing x indices for which plots of time-resolved spectra are desired under a spectral model

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`opt-class`, `kinopt-class`

`sumKinSpecEst`	*Makes a summary plot of spectra associated with kinetic components alongside a plot showing parameter estimates*

Description

Makes a summary plot of spectra associated with kinetic components alongside a plot showing parameter estimates for, by default, kinetic parameters. If the analysis had more parameters in the `addEst` slot of the arguement `opt`, then more parameters are displayed. Note that this summary leaves out the spectra associated with coherent artifact or scatter.

Usage

```
sumKinSpecEst(listFits, addtitle = TRUE, customtitle = "", preps = "",
ylimlist=list(), kinspecerr=TRUE)
```

Arguments

`listFits`	list of objects returned by the `fitModel` function
`addtitle`	logical regarding whether to add a title; if TRUE and `customtitle` is not given then the title is `"Summary of EADS for:  "` plus the analysis titles
`customtitle`	character vector containing a title
`preps`	character vector describing the prefix of the postscript filename given as output
`ylimlist`	list with elements `list(ind, ylim)`. `ind` is an index into `listFits`; `ylim` is the desired `ylim` for the plot for that analysis
`kinspecerr`	logical regarding whether to add error bars for to the estimated spectra.

Details

This looks best with less than five objects in `listFits`.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

`fitModel`, `examineFit`

theta-class	*Class "theta" for storage of nonlinear parameter estimates*

Description

theta is the class to store parameter estimates associated with possibly many datasets; after a call to fitModel a list containing theta objects for each of the n datasets analyzed in the call to fitModel is created. To see the parameter estimates associated with the datasets, examine the object currTheta in the list returned by fitModel

Details

after a call to fitModel, an object of class theta exists in the global environment as the variable currTheta

Objects from the Class

Objects can be created by calls of the form new("theta", ...) or theta(...).

Slots

kinpar: Object of class "vector" of rate constant estimates

specpar: Object of class "list" of spectral shape parameter estimates

irfpar: Object of class "vector" of IRF parameter estimates

parmu: Object of class "list" of parameter estimates describing dispersion of the location of other parameters (in time, temp., etc.)

partau: Object of class "vector" of parameter estimates describing dispersion of the width of other parameters (in time)

clpequ: Object of class "vector" of parameter estimates describing conditionally linear parameters (spectra, in a kinetic model) relations

specdisppar: Object of class "list" of parameter estimates describing dispersion of spectra

kinscal: Object of class "vector" of parameters describing kinetic relations in the context of a compartmental scheme

prel: Object of class "vector" of parameters describing relations between parameters (which may be linear, exponential, etc.)

coh: Object of class "vector" of parameters describing a coherent artifact or pulse follower.

drel: Object of class "vector" of parameters describing relations between datasets (linear, and possibly per-wavelength or, in general, per-clp)

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

fitModel , multitheta-class

TIMP-package | *a problem solving environment for fitting separable nonlinear models in physics and chemistry applications*

Description

TIMP is a problem solving environment for fitting separable nonlinear models to measurements arising in physics and chemistry experiments, and has been extensively applied to time-resolved spectroscopy and FLIM-FRET data.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum Maintainer: Katharine M. Mullen ⟨kate@nat.vu.nl⟩

References

Mullen KM, van Stokkum IHM (2007). "TIMP: An R Package for Modeling Multi-way Spectroscopic Measurements." Journal of Statistical Software, 18(3). URL http://www.jstatsoft.org/v18/i03/.

Laptenok S, Mullen KM, Borst JW, van Stokkum IHM, Apanasovich VV, Visser AJWG (2007). "Fluorescence Lifetime Imaging Microscopy (FLIM) Data Analysis with TIMP." Journal of Statistical Software, 18(8). URL http://www.jstatsoft.org/v18/i08/.

See http://timp.r-forge.r-project.org/ or http://www.nat.vu.nl/~kate/TIMP/ for further documentation.

---

writeAverage | *Writes the average of scans stored in a file to a new file in the 'ivo' format*

Description

Some measurement set-ups dump a set of matrices stacked on top of each other to a file; each matrix represents a scan. This function writes the average of the scans to a file in the '.ivo' format.

Usage

```
writeAverage(filename, ntimes, nwave, scans,
             fileout = paste(filename, "Average.ivo", sep=""),
             calibration = 1:nwave, wexplicit=FALSE)
```

Arguments

`filename`	This is the path to the file to read in, as a quoted string.
`ntimes`	number of times in each scan
`nwave`	number of wavelengths in each scan
`scans`	number of full scans to read
`fileout`	a character vector specifying the filename to write the averaged data to; the default is to write a file named "filenameAverage.ivo"
`calibration`	a numeric vector representing the wavelength labels; by default the labels "1, 2, ..., nwave" are used
`wexplicit`	logical whether the file is written in the 'wavelength explicit' format, with each column of the matrix written representing a wavelength, as opposed to the 'time explicit' format, where each column represents a timepoint.

Author(s)

Katharine M. Mullen, Ivo H. M. van Stokkum

See Also

readData

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