Package 'albatross'

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Type Package

Title PARAFAC Analysis of Fluorescence Excitation-Emission Matrices

Version 0.3-7

Depends R (>= 3.3)

Imports multiway (>= 1.0-4), CMLS, pracma, lattice, parallel, Matrix

Enhances eemR, EEM

Description Perform parallel factor analysis (PARAFAC: Hitchcock, 1927) <doi:10.1002/sapm192761164> on fluorescence excitation-emission matrices: handle scattering signal and inner filter effect, scale the dataset, fit the model; perform split-half validation or jack-knifing. Modified approaches such as Whittaker interpolation, randomised split-half, and fluorescence and scattering model estimation are also available. The package has a low dependency footprint and has been tested on a wide range of R versions.

License GPL (>= 3)

BuildResaveData no

BuildManual yes

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albatross-package   *PARAFAC Analysis of Fluorescence Excitation-Emission Matrices*

Description

> Day after day, day after day,
> We stuck, nor breath nor motion;
> As idle as a painted ship
> Upon a painted ocean.
>
> Water, water, every where,
> And all the boards did shrink;
> Water, water, every where,
> Nor any drop to drink.

> – Samuel Taylor Coleridge, *The Rime of the Ancient Mariner*

Perform parallel factor analysis (PARAFAC: Hitchcock, 1927) <doi:10.1002/sapm192761164> on fluorescence excitation-emission matrices: handle scattering signal and inner filter effect, scale the dataset, fit the model; perform split-half validation or jack-knifing. Modified approaches such as Whittaker interpolation, randomised split-half, and fluorescence and scattering model estimation are also available. The package has a low dependency footprint and has been tested on a wide range of R versions.

Details

In order to work with your data, create feem and/or feemcube objects from files or matrix or array objects. Use feemlist to import files in bulk. If your files aren't in one of the formats supported by feem but you can read their contents by other means, you can supply an importer function to feemlist; it should take a file name and return the corresponding feem object.

Operations that can be performed on the objects include plotting (plot.feem), calculation of fluorescence indices (feemindex), inner-filter effect correction (feemife), handling of scattering signal (feemscatter), changing the wavelength grid of the data by means of interpolation (feemgrid), and scaling (feemscale). Scaling may be automatically undone after performing the PARAFAC decomposition so that the resulting scores would correspond to the data as it was before the scaling.

All processing functions can take individual feem objects, lists of them, or feemcube objects and return values of the appropriate kind. For example, feemscatter always returns an object of the same class but with the scattering signal handled, while feemindex returns named numeric vectors for individual feems but data.frames for collections of them. There's a slight memory benefit to using lists of feem objects, but the difference shouldn't be noticeable, so there's nothing to worry about if you started with a feemcube.

In order to compute PARAFAC, you need to convert your data into a feemcube. Whether you perform jack-knifing, split-half analysis, or PARAFAC itself, a copy of the data cube is kept together with the results and can be extracted back using the feemcube function. The resulting objects support a plot method (described in the same help page) and can give you the data as a few-column data.frame using the coef method.

Once the analysis is finished, the PARAFAC model can be exported for the OpenFluor database (`write.openfluor`) or stored as an R object using standard R tools (`save` or `saveRDS`).

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write.openfluor         Export a PARAFAC model for the OpenFluor
                        database
```

Author(s)

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References

Murphy KR, Stedmon CA, Graeber D, Bro R (2013). "Fluorescence spectroscopy and multi-way techniques. PARAFAC." *Analytical Methods*, **5**, 6557-6566. doi:10.1039/c3ay41160e.

Pucher M, Wünsch U, Weigelhofer G, Murphy K, Hein T, Graeber D (2019). "staRdom: Versatile Software for Analyzing Spectroscopic Data of Dissolved Organic Matter in R." *Water*, **11**(11), 2366. doi:10.3390/w11112366.

Cleese J, Jones T (1970). "Albatross: Flavours of different sea birds." *Journal of Flying Circus*, **1.13**, 7:05-7:45.

Krylov I, Drozdova A, Labutin T (2020). "Albatross R package to study PARAFAC components of DOM fluorescence from mixing zones of arctic shelf seas." *Chemometrics and Intelligent Laboratory Systems*, **207**(104176). doi:10.1016/j.chemolab.2020.104176.

See Also

feem, feemlist, feemindex, feemife, feemscatter, feemgrid, feemcube, feemscale, feemsplithalf, feemparafac, feemjackknife, feemflame, absindex.

Examples

```
data(feems)

dataset <- feemcube(feems, FALSE)
dataset <- feemscatter(dataset, rep(24, 4), 'pchip')
dataset <- feemife(dataset, absorp)
plot(dataset <- feemscale(dataset, na.rm = TRUE))


  # takes a long time
  (sh <- feemsplithalf(cube, nfac = 2:5, splits = 4))
  plot(sh)
  jk <- feemjackknife(cube, nfac = 3)
  plot(jk)


pf <- feemparafac(cube, nfac = 3)
plot(pf)
```

---

absindex   *Functions of absorbance data*

Description

Calculate absorption coefficients and/or absorbance data at given wavelengths, spectral slopes, and their ratios.

Usage

```
absindex(
  x, abs.path, unit = c("log10", "m^-1"), out.A = 254,
  out.a = c(350, 355, 374, 443),
  out.a.ratio = list(c(250, 365), c(465, 665)),
  out.slope = list(c(275, 295), c(350, 400)),
  out.slope.ratio = list(c(275, 295, 350, 400)),
  out.slope.nrmse = FALSE
)
```

Arguments

x
:   Absorption data, either a list of two-column matrix-like objects with wavelengths in first column and values in second column, or a multi-column matrix-like object with wavelengths in first column and values in all other columns. Can be named in order to match with the abs.path values, see feemife for details.

abs.path
:   A numeric vector of optical path lengths for every spectrum, in centimetres. Defaults to 1 for all samples. If specified, should be either named, with names matching x, or unnamed and containing exactly the same number of path lengths.

unit	Specifies whether x contains absorbance (`log10`; $A = \log_{10}\frac{I_0}{I}$; unitless) or absorption coefficients (`m^-1`; $\alpha = \frac{\ln\frac{I_0}{I}}{l}$; $[\mathrm{m}^{-1}]$).
out.A	Return absorbance values at the wavelengths given as a numeric vector.
out.a	Return absorption coefficients at the wavelengths given as a numeric vector.
out.a.ratio	Return ratios of absorption coefficients at the wavelengths given as a list of two-element numeric vectors. For every pair of wavelengths, $\frac{\alpha(\lambda_1)}{\alpha(\lambda_2)}$ is returned.
out.slope	Return spectral slopes at wavelength ranges given as a list of two-element numeric vectors. See the `slope.method` for the description of how spectral slopes are computed.
out.slope.ratio	
	Return ratios of spectral slopes for pairs of wavelength ranges given as a list of four-element numeric vectors. For every list element, the value returned is $\frac{S(\lambda_1,\lambda_2)}{S(\lambda_3,\lambda_4)}$.
out.slope.nrmse	
	When computing slopes, also return the root-mean-square error for the models providing them, divided by the range of the response: $\frac{1}{y_{\max}-y_{\min}}\sqrt{\sum_{i=1}^{n}\frac{(\hat{y}_i-y_i)^2}{n}}$.

Details

Currently, the spectral slopes are calculated by fitting a linear model $\ln\alpha = b_0 - b_1\lambda$ and returning b_1 as the slope. See (Twardowski, Boss, Sullivan, and Donaghay 2004) for a discussion of the calculation methods for spectral slopes.

Requested wavelengths missing from the original grid are interpolated using [spline](). NA values are returned outside the original wavelength range.

Value

A [data.frame]() with one row per sample, containing the following columns:

sample	Names or numbers of the samples.
A.<wavelength>	Absorbance values, for every *wavelength* in `out.A`.
a.<wavelength>	Absorption coefficients, for every *wavelength* in `out.a`.
aR.<wl[1]>.<wl[2]>	
	Ratios of absorption coefficients, for every *wl* in `out.a.ratio`.
S.<wl[1]>.<wl[2]>	
	Spectral slopes, for every *wl* in `out.slope`.
NRMSE.S.<wl[1]>.<wl[2]>	
	If `out.slope.nrmse` is TRUE, root-mean-square errors normalised by the range of the absorption coefficients for the models providing spectral slopes.
SR.<wl[1]>.<wl[2]>.<wl[3]>.<wl[4]>	
	Ratios of spectral slopes, for every *wl* in `out.slope.ratio`.

References

Twardowski MS, Boss E, Sullivan JM, Donaghay PL (2004). "Modeling the spectral shape of absorption by chromophoric dissolved organic matter." *Marine Chemistry*, **89**(1), 69-88. doi:10.1016/j.marchem.2004.02.008.

See Also

[feemife](#)

Examples

```
data(feems)
absindex(absorp)
```

---

as.data.frame.feem   *Transform a FEEM object into a data.frame*

Description

Transform a FEEM object from its matrix form accompanied by vectors of wavelengths into a three-column form consisting of $(\lambda_{em}, \lambda_{ex}, I)$ tuples, which could be useful for export or plotting with **lattice** or **ggplot2**.

Usage

```
## S3 method for class 'feem'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)
## S3 method for class 'feemcube'
as.data.frame(x, ...)
```

Arguments

x	A FEEM object, or a FEEM cube object.
row.names	Passed to [data.frame](#). If default of NULL is used, [data.frame](#) will generate sequential integer row.names.
optional	This option is required for compatibility with [as.data.frame](#) generic, but is ignored, since the column names are already syntactic and the row names are generated by [data.frame](#) automatically by default.
...	Passed as-is to [data.frame](#).

Details

Rows where intensity is NA are omitted from the output.

Value

A [data.frame](#) containing three numeric columns:

emission	Emission wavelength, nm.
excitation	Excitation wavelength, nm.
intensity	Fluorescence intensity at $(\lambda_{em}, \lambda_{ex})$
sample	For FEEM cube objects, the unique name of the sample possessing this tuple of values, a factor. If the original object didn't have any names, sequential integers are used instead. If the original object had non-unique names, sequence numbers are appended to them using [make.unique](#).

See Also

[feem.data.frame](#)

Examples

```
z <- feem(matrix(1:42, nrow = 7), 1:7, 1:6)
head(as.data.frame(z))
```

---

feem   *Create a fluorescence excitation-emission matrix object*

Description

Functions to create fluorescence excitation-emission matrix objects from R matrices coupled with excitation and emission wavelengths, three-column data.frames containing $(\lambda_{em}, \lambda_{ex}, I)$ tuples or files.

Usage

```
feem(x, ...)
  ## S3 method for class 'matrix'
feem(x, emission, excitation, scale = 1, ...)
  ## S3 method for class 'data.frame'
feem(
    x, scale = 1, emission = 'emission',
    excitation = 'excitation', intensity = 'intensity', ...
  )
  ## S3 method for class 'character'
feem(x, format, ...)
  ## S3 method for class 'connection'
feem(x, format, ...)
```

Arguments

x
: The source of the information to create a FEEM object from: a matrix, a three-column data.frame, a file path as a single string, or a [connection](#).

  If converting a matrix, its rows should correspond to different fluorescence emission wavelengths specified in the emission argument; conversely, its columns should correspond to excitation wavelengths specified in the excitation argument.

  If converting a data.frame, it should have exactly three columns containing emission wavelengths, excitation wavelength, and intensity values. The names of the columns are expected to be "emission", "excitation", and "intensity", respectively, but can be overridden using namesake arguments.

  If reading a single file by file path or connection, the format argument must specify the kind of file to parse, see below.

emission
: If converting a matrix, this should be a vector of emission wavelengths, each wavelength corresponding to a row of the matrix.

  If converting a data.frame, this optional argument specifies the name of the column containing the emission wavelengths.

excitation	If converting a matrix, this should be a vector of excitation wavelengths, each wavelength corresponding to a column of the matrix.
	If converting a `data.frame`, this optional argument specifies the name of the column containing the excitation wavelengths.
intensity	If converting a `data.frame`, this optional argument specifies the name of the column containing the fluorescence intensities.
scale	The scale value of a EEM is preserved through the analysis procedure to divide the resulting score values after running PARAFAC. If the EEM has been pre-multiplied prior to creating the FEEM object, you can set the multiplier here.
format	**table** The FEEM is assumed to be stored as a plain text matrix, readable using read.table, with the first column and the first row containing wavelengths. For example, it is possible to import CSV files obtained from a HORIBA Aqualog® fluorometer by using feem(*file*, 'table', sep = ',').

     Rows are assumed to correspond to emission wavelengths, columns are assumed to correspond to excitation wavelengths; if that's not the case, set the `transpose` argument to `TRUE`.

     If there are unmeasured points in the spectrum (e.g. the anti-Stokes area) but they are hard to distinguish from measured values (e.g. stored as zeroes instead of NA), specify their values as the `na` argument (numeric vector). The function will check for triangles filled with these values (such that a threshold Δ exists where for all $\lambda_{em} - \lambda_{ex} > \Delta$ or $\lambda_{em} - \lambda_{ex} < \Delta$, $X(\lambda_{em}, \lambda_{ex}) \in$ `na`) and replace them with NAs. If the unmeasured values are not stored as numbers, use the `na.strings` argument of read.table to specify them.

     The `fileEncoding` argument is treated specially (but preserving the read.table semantics regarding numbers), preventing errors in case the session charset cannot represent all characters from the file: the contents are first converted to UTF-8, then forwarded to read.table. This only works when `file` is a file path, not a connection. (When passing a connection with an encoding attribute set, make sure that the file contents after decoding can be represented in the session charset.)

     All other arguments are passed to read.table, with `fill` defaulting to `TRUE` instead of `FALSE`.

panorama Read a '.dat' file as created by "Panorama" software that comes with FLUORAT®-02-PANORAMA fluorometer. Such files contain a header describing the wavelength range, e.g.:

```
240.0   650.0    1.0    ; Emission(columns)
230.0   320.0    5.0    ; Excitation(rows)
```

     The header is followed by the intensity data as matrix, whitespace-separated. Missing points (anti-Stokes area) stored as 0 or 100 and are automatically filtered out on import. No additional parameters are accepted.

F900txt Read an emission map text file created by "F900" software that comes with Edinburgh Instruments fluorescence spectrometers. Separated by empty lines, these files are assumed to contain:

1. Sample name
2. Metadata of each emission scan, with names in the first column, including the excitation wavelengths
3. Fluorescence values with emission wavelengths in the first column

     The `fileEncoding` argument specifies the encoding of the text file and has a safe default of "latin1". It should typically correspond to the ANSI code

page on the computer running F900 that was used to create the file. See [iconvlist](.)() for a list of encodings understood by R.

The sep argument specifies the column separator used in the file. A semicolon ; is typically used, though other options are possible.

...   When converting matrices and [data.frame](.)s, extra arguments besides those specified above are not allowed.

When reading the FEEM from a file, additional arguments may be passed to format-specific reading functions, see above.

Details

Transposing a feem object using [t](.) will remove the class attribute, returning an ordinary matrix.

Value

A FEEM object is a matrix with the following attributes added:

emission   Fluorescence emission wavelengths corresponding to the rows of the matrix, nm.

excitation   Fluorescence excitation wavelengths corresponding to the columns of the matrix, nm.

dimnames   Dimension names, copies of information above. Used only for presentation purposes.

scale   Scale factor, preserved through the analysis, which may be used later to undo the scaling. Initially 1.

See Also

FEEM methods: [plot.feem](.), [as.data.frame.feem](.), [\[.feem](.), [feemgrid](.), [feemife](.), [feemscale](.), [feemscatter](.).

Examples

```
feem(matrix(1:40, ncol = 8), 1:5, 1:8)
feem(
  data.frame(x = 1:10, y = 21:30, z = 31:40),
  emission = 'x', excitation = 'y', intensity = 'z'
)
feem(
  system.file('extdata/ho_aq.csv', package = 'albatross'),
  'table', sep = ','
)
feem(
  system.file('extdata/F900.txt', package = 'albatross'), 'F900txt'
)
```

---

feemcube *Data cubes of fluorescence excitation-emission matrices*

Description

Given a list of [feem](#) objects or a 3-way array, build tagged 3-dimensional arrays of fluorescence excitation-emission spectra. Extract the data cube from the corresponding model objects. Transform the data cube into a list of [feem](#) objects.

Usage

```
  feemcube(x, ...)
  ## S3 method for class 'list'
feemcube(x, all.wavelengths, ...)
  ## S3 method for class 'array'
feemcube(x, emission, excitation, scales, names = NULL, ...)
  ## S3 method for class 'feemparafac'
feemcube(x, ...)
  ## S3 method for class 'feemsplithalf'
feemcube(x, ...)
  ## S3 method for class 'feemjackknife'
feemcube(x, ...)
  ## S3 method for class 'feemflame'
feemcube(x, ...)
  ## S3 method for class 'feemcube'
as.list(x, ...)
```

Arguments

x	**feemcube** A list of FEEM objects, possibly named, or a numeric array. Alternatively, a [feemparafac](#), [feemjackknife](#), [feemsplithalf](#), or a [feemflame](#) object.
	as.list.feemcube A feemcube object.
all.wavelengths	
	Logical, a flag specifying whether to include wavelengths not present in *all* of the samples. If FALSE, only those wavelength present in all of the samples are included.
emission	Numeric vector of emission wavelengths. Should correspond to the first dimension of the array x.
excitation	Numeric vector of excitation wavelengths. Should correspond to the second dimension of the array x.
scales	Numeric vector of scale factors corresponding to the spectra in the array. Should correspond to the third dimension of the array x. If missing, assumed to be all 1.
names	Character vector of names of the samples. Should correspond to the third dimension of the array x.
...	Additional arguments besides those specified above are not allowed.

Details

feemcube.list can be used to build FEEM data cubes from lists of FEEM objects even if their wavelength grids do not exactly match. The missing wavelengths may be set to NA (all.wavelengths = TRUE) or omitted from the cube (all.wavelengths = FALSE). See [feemgrid](#) if you need to adjust the wavelength grid of a list of EEMs before making it into a FEEM cube.

feemcube.feemparafac, feemcube.jackknife, and feemcube.feemsplithalf return the data cube originally passed to the corresponding functions.

Value

A FEEM data cube is a numeric three-dimensional array with the following attributes:

emission	Fluorescence emission wavelengths corresponding to the first dimension of the array, nm.
excitation	Fluorescence excitation wavelengths corresponding to the second dimension of the array, nm.
dimnames	Dimension names, copies of information above. Used only for presentation purposes.
scales	Scale factors of the samples, corresponding to the third dimension of the array. Assumed to be 1 if not specified by the user.

as.list.feemcube: A named list of FEEM objects comprising x.

See Also

FEEM cube methods: [`[.feemcube`](#), [`plot.feemcube`](#), [`as.data.frame.feemcube`](#), [`feemife`](#), [`feemscale`](#), [`feemscatter`](#).

Examples

```
# array form
feemcube(
  array(1:24, c(4, 3, 2)), # 3-way array obtained elsewhere
  seq(340, 400, len = 4), seq(250, 300, len = 3) # wavelengths
)
# list form
feemcube(
  replicate(2, feem( # list of feem objects
    matrix(1:6, 2), c(340, 400), c(250, 275, 300)
  ), FALSE),
  TRUE
)
str(as.list(feemcube(array(1:60, 3:5), 1:3, 1:4)))
```

---

feemflame	*Fluorescence and scAttering Model Estimation*

Description

Given a FEEM cube, model the fluorescence and the scattering signals at the same time as a sum of a PARAFAC model and a low-rank unfolded matrix factorisation.

Usage

```
    feemflame(
      X, ffac, sfac, maxiter = 32, widths = rep(25, 4), Raman.shift = 3400,
      ctol = 1e-04, progress = TRUE
    )
    ## S3 method for class 'feemflame'
  fitted(object, ...)
    ## S3 method for class 'feemflame'
  residuals(object, ...)
    ## S3 method for class 'feemflame'
  coef(
      object, type = c(
        "fluorescence",
        "scores", "loadings", "emission", "excitation", "samples",
        "scattering", "sc.scores", "sc.loadings"
      ), ...
    )
    ## S3 method for class 'feemflame'
  plot(
      x, type = c('both', 'fl.image', 'fl.lines'), ...
    )
```

Arguments

X	A [feemcube](#) object.
ffac	The number of trilinear components used to model fluorescence, passed to [feemparafac](#).
sfac	The number of bilinear (low-rank matrix factorisation) components used to model the scattering signal.
maxiter	Maximum number of alternating PARAFAC and constrained matrix factorisation iterations.
widths	Widths of the scattering regions, like in [feemscatter](#): A numeric vector of length 4 containing the widths (in nm) of the scattering signal, in the following order:

1. Rayleigh scattering
2. Raman scattering
3. Rayleigh scattering, 2λ
4. Raman scattering, 2λ

Raman.shift	Raman shift of the scattering signal, in cm^{-1}, like in [feemscatter](#).
ctol	Given $L = \|\mathbf{X} - \hat{\mathbf{X}}\|^2$, stop when $\frac{|\Delta L|}{L} \leq$ `ctol`.
progress	Print progress information on the console, including the iteration number, relative sum of squared residuals, and relative change in sum of squared residuals.
object, x	A `feemflame` object.
type	**coef** Determines the type of coefficients to return: **fluorescence** Equivalent to calling [coef.feemparafac](#) on the fluorescence model (default). **scores, loadings, emission, excitation, samples** Equivalent to calling [coef.feemparafac](#) on the fluorescence model and passing the respective type argument. **sc.scores** A [data.frame](#) containing the following columns:

>>> **sample** Sample numbers or names.
>>> **value** Scattering intensity value for a given factor.
>>> **factor** The number of the scattering component.
>> **sc.loadings** A [data.frame](#) containing the following columns:
>>> **emission, excitation** The wavelengths corresponding to the value of the scattering profile.
>>> **value** Scattering intensity value for a given factor.
>>> **factor** The number of the scattering component.
>> **scattering** A list with names "scores" and "loadings" containing results of `coef(object, 'sc.scores')` and `coef(object, 'sc.loadings')`, respectively.
> **plot** Describes the kind of plot to produce:
>> **both** Plot the loadings of the fluorescence and scattering models as false colour images.
>> **fl.image, fl.lines** Equivalent to calling [plot.feemparafac](#) on the fluorescence model with the argument "image" or "lines", respectively.
> `...` No other parameters are allowed.

Details

FLAME models the input data as a sum of fluorescence signal (PARAFAC model) and scattering signal (low rank model):

$$X_k(\lambda_i^{\mathrm{em}}, \lambda_j^{\mathrm{ex}}) = \underbrace{\sum_p A_{i,p} B_{j,p} C_{k,p}}_{\text{fluorescence}} + \underbrace{\sum_q S_{i,j,q} D_{k,q}}_{\text{scattering}}$$

The function alternates between fitting the PARAFAC model on the dataset with scattering signal subtracted and fitting the low-rank model on the dataset with fluorescence signal subtracted. The PARAFAC model is fitted using the [feemparafac](#) function. The low-rank model is fitted by means of unfolding the wavelength dimensions into one, resulting in a matrix, followed by the same alternating least squares procedure as done in multivariate curve resolution. Both models are constrained to result in non-negative factors.

The low-rank model is additionally constrained to zero outside the scattering region. The scattering region is defined the same way as in [feemscatter](#), using the `widths` and the `Raman.shift` arguments.

Initial PARAFAC model is fitted with the scattering region set to missing. The low-rank model is initialised with truncated singular value decomposition forced to be non-negative.

Value

`feemflame` An object of class `feemflame`, which is a list containing the following components:
> **fl** A [feemparafac](#) object containing the fluorescence part of the model.
> **sc** An object of internal class `cmf`. Please don't rely on its structure.

`fitted.feemflame`
> A [feemcube](#) object containing the part of X fitted by the model.

`residuals.feemparafac`
> A [feemcube](#) object equal to $\mathbf{X} - \hat{\mathbf{X}}$, with an extra class `feem.resid` set. Objects of this class are plotted with a different default palette, see [plot.feem.resid](#).

`coef.feemflame` See the description of the `type` argument.

Note

The structure of the `feemflame` object, the initialisation, and the constraints may be subject to change in a future version.

References

Tauler R, Marqués I, Casassas E (1998). "Multivariate curve resolution applied to three-way trilinear data: Study of a spectrofluorimetric acid-base titration of salicylic acid at three excitation wavelengths." *Journal of Chemometrics*, **12**(1), 55-75. doi:10.1002/(SICI)1099128X(199801/02)12:1<55::AIDCEM501>3.0.CO;2#.

Krylov I, Labutin T, Rinnan Å, Bro R (2021). "Modelling of scattering signal for direct PARAFAC decompositions of excitation-emission matrices." 17th Scandinavian Symposium on Chemometrics. https://web.archive.org/web/20220314144225/https://ssc17.org/abstract/Krylov1.html. https://files.libs.chem.msu.ru/~ivan/SSC17/P13.pdf.

See Also

feemparafac, feemcube

Examples

```
data(feems)
cube <- feemscale(cube)
factors <- feemflame(cube, ffac = 3, sfac = 1)
str(coef(factors))
str(coef(factors, 'scattering'))
plot(factors)
```

---

feemgrid   *Interpolate FEEMs on a given wavelength grid*

Description

Use interpolation to change the wavelength grid of a single FEEM or unify the grid of a collection of them.

Usage

```
feemgrid(x, ...)
  ## S3 method for class 'feem'
feemgrid(
    x, emission, excitation,
    method = c("whittaker", "loess", "kriging", "pchip"), ...
  )
  ## S3 method for class 'feemcube'
feemgrid(
    x, emission, excitation, ..., progress = TRUE
  )
  ## S3 method for class 'list'
feemgrid(
    x, emission, excitation, ..., progress = TRUE
  )
```

Arguments

x	A feem object, a feemcube, or a list of feem objects.
emission, excitation	
	Desired wavelength grid, as numeric vectors. Must be specified for a single FEEM. If not specified for a collection of FEEMs, all wavelengths falling in the range of the intersection all wavelengths intervals are chosen.
method	Interpolation method, see feemscatter for details.
...	Passed from generics to feemgrid.feem, then to interpolation methods. See feemscatter for details.
progress	Set to FALSE to disable the progress bar.

Details

The algorithm doesn't know how to distinguish between NAs that haven't been measured and NAs that resulted from combining different wavelength grids, so it tries to interpolate all of them. As a result, leaving large areas of the spectrum undefined (e.g. anti-Stokes area) is not recommended, since it would result in extrapolation and introduce strong artefacts.

Value

An object of the same kind (FEEM object / FEEM cube / list of them) with emission and excitation wavelengths as requested.

See Also

feemscatter

Examples

```
data(feems)
x <- feemscatter(feems$a, rep(25, 4))
y <- feemgrid(x, seq(240, 600, 5), seq(230, 550, 10))
plot(plot(x, main = 'Original'    ), split = c(1, 1, 2, 1), more = TRUE)
plot(plot(y, main = 'Interpolated'), split = c(2, 1, 2, 1))
```

---

feemife   *Absorbance-based inner filter effect correction*

Description

Use absorbance data to correct inner-filter effect in FEEM objects and collections of them.

Usage

```
feemife(x, ...)
  ## S3 method for class 'feem'
feemife(x, absorbance, abs.path = 1, ...)
  ## S3 method for class 'feemcube'
feemife(x, absorbance, abs.path, ..., progress = FALSE)
  ## S3 method for class 'list'
feemife(x, absorbance, abs.path, ..., progress = FALSE)
```

Arguments

x	A FEEM object, a FEEM data cube, or a list of them.
absorbance	If x is a FEEM object: a two-column matrix-like object containing the absorbance spectrum of the sample: the wavelengths in the first column and the unitless absorbance values in the second column.
	Otherwise, this could be a list of such objects or a multi-column matrix-like object. If x contains names of the samples (is a named list or had names specified when calling [feemcube](#)), absorbance is a named list or has named columns, and all samples from x can be looked up in absorbance, results of this lookup are used. If x or absorbance isn't named, but (given N-sample x) absorbance has exactly $N + 1$ columns or is an N-element list, absorbance spectra are assumed to be present in the same order as the samples in x. Otherwise, an error is raised.
abs.path	If x is a FEEM object, a number specifying the length of the optical path used when measuring the absorbance, cm.
	Otherwise, a named vector containing the names from x, or a vector of exactly same length as the number of FEEMs in x: same lookup rules apply as for absorbance argument.
	If not set, assumed to be 1.
progress	Set to TRUE to enable a progress bar (implemented via [txtProgressBar](#)).
...	No parameters besides those described above are allowed.

Details

If you receive errors alleging that some names don't match, but are absolutely sure that the absorbance spectra and path lengths are present in the same order as in x, remove the names from either of the objects, e.g. by passing [unname](#)(absorbance).

The formula used to correct for inner filter effect is:

$$I_{\text{corr}}(\lambda_{\text{em}}, \lambda_{\text{ex}}) = I_{\text{orig}}(\lambda_{\text{em}}, \lambda_{\text{ex}}) 10^{\frac{A(\lambda_{\text{em}}) + A(\lambda_{\text{ex}})}{2L_{\text{abs}}}}$$

Value

An object of the same kind as x, with inner filter effect corrected.

References

Lakowicz JR (2006). *Principles of Fluorescence Spectroscopy, 3rd ed.*. Springer US. doi:10.1007/9780387463124.

Kothawala DN, Murphy KR, Stedmon CA, Weyhenmeyer GA, Tranvik LJ (2013). "Inner filter correction of dissolved organic matter fluorescence." *Limnology and Oceanography: Methods*, **11**(12), 616-630. doi:10.4319/lom.2013.11.616.

Examples

```
data(feems)

str(cube)
str(absorp)
plot(feemife(cube,absorp) / cube)
```

---

feemindex   *Fluorescence indices and peak values*

Description

Calculate fluorescence indices or peak values for individual FEEMs or groups of them.

Usage

```
  feemindex(x, ...)
  ## S3 method for class 'feem'
feemindex(
    x,
    indices = c(
      "HIX", "BIX", "MFI", "CFI", "YFI", "FrI",
      "A", "B", "C", "M", "P", "T"
    ),
    tolerance = 1, interpolate = FALSE, ...
  )
  ## S3 method for class 'feemcube'
feemindex(x, ..., progress = FALSE)
  ## S3 method for class 'list'
feemindex(x, ..., progress = FALSE)
```

Arguments

x	A FEEM, a FEEM cube, or a list of [feem](#) objects.
indices	Fluorescence indices or peaks to return. By default, all indices and peaks known to the function are returned. See Details for their meaning.
tolerance	A numeric scalar signifying the acceptable emission and excitation wavelength error in nm. For example, if a wavelength of 254 nm is needed to calculate an index, a value at 255 nm can be considered if tolerance >= 1. Defaults to 1 nm. See below for what happens if no matching value is found.
interpolate	A string specifying an interpolation method ("whittaker", "loess", "kriging", "pchip"), or FALSE to disable interpolation (default).
	If interpolation is disabled, an index will get an NA value when required points are too far from the measured grid or are present in the grid but set to NA.
	When interpolation is enabled, required points that are missing from the grid or present but set to NA will be interpolated using [feemgrid](#) as long as they are within the wavelength bounds of the FEEM. NAs may still be returned only when the desired value is impossible to interpolate due to it being outside the wavelength range.
...	Additional parameters eventually passed to interpolation methods. See [feemscatter](#) for details.
progress	Set to TRUE to enable a progress bar (implemented via [txtProgressBar](#)).

Details

Available indices and peaks are:

HIX

$$\mathrm{HIX} = \frac{\int_{435\,\mathrm{nm}}^{480\,\mathrm{nm}} I \, d\lambda_{\mathrm{em}}}{\int_{300\,\mathrm{nm}}^{345\,\mathrm{nm}} I \, d\lambda_{\mathrm{em}}} \text{ at } \lambda_{\mathrm{ex}} = 254\,\mathrm{nm}$$

Higher values of the humification index correspond to more condensed fluorescing molecules (higher C/H), more humified matter. (Zsolnay, Baigar, Jimenez, Steinweg, and Saccomandi 1999)

BIX

$$\mathrm{BIX} = \frac{I(\lambda_{\mathrm{em}} = 380\,\mathrm{nm})}{I(\lambda_{\mathrm{em}} = 430\,\mathrm{nm})} \text{ at } \lambda_{\mathrm{ex}} = 310\,\mathrm{nm}$$

Index of recent autochthonous contribution determines the presence of the β fluorophore, characteristic of autochthonous biological activity in water samples. (Huguet, Vacher, Relexans, Saubusse, Froidefond, and Parlanti 2009)

MFI

$$\mathrm{MFI} = \frac{I(\lambda_{\mathrm{em}} = 450\,\mathrm{nm})}{I(\lambda_{\mathrm{em}} = 500\,\mathrm{nm})} \text{ at } \lambda_{\mathrm{ex}} = 370\,\mathrm{nm}$$

The fluorescence index by (McKnight, Boyer, Westerhoff, Doran, Kulbe, and Andersen 2001) helps distinguish sources of isolated aquatic fulvic acids and may indicate their aromaticity.

CFI

$$\mathrm{CFI} = \frac{I(\lambda_{\mathrm{em}} = 470\,\mathrm{nm})}{I(\lambda_{\mathrm{em}} = 520\,\mathrm{nm})} \text{ at } \lambda_{\mathrm{ex}} = 370\,\mathrm{nm}$$

The fluorescence index by (Cory and McKnight 2005) is correlated to relative contribution of microbial versus higher plant-derived organic matter to the DOM pool.

YFI

$$\mathrm{YFI} = \frac{\bar{I}(\lambda_{\mathrm{em}} \in [350, 400]\,\mathrm{nm})}{\bar{I}(\lambda_{\mathrm{em}} \in [400, 450]\,\mathrm{nm})} \text{ at } \lambda_{\mathrm{ex}} = 280\,\mathrm{nm}$$

Yeomin fluorescence index (Heo, Yoon, Kim, Lee, Lee, and Her 2016) is lowest for humic-like and fulvic-like samples, higher for aminosugar-like samples and highest for protein-like samples.

FrI

$$\mathrm{FrI} = \frac{I(\lambda_{\mathrm{em}} = 380\,\mathrm{nm})}{\max I(\lambda_{\mathrm{em}} \in [420, 435]\,\mathrm{nm})} \text{ at } \lambda_{\mathrm{ex}} = 310\,\mathrm{nm}$$

The freshness index, also known as $\frac{\beta}{\alpha}$, is an indicator of autochthonous inputs (Wilson and Xenopoulos 2009) and may provide indication of relative contribution of microbially produced DOM.

A, B, C, M, P, T Fluorophore peaks taken from (Coble 2007):

Peak	λ_{ex}	λ_{em}	Fluorescence
A	260	400-460	humic-like
B	275	305	tyrosine-like
C	320-360	420-460	humic-like
M	290-310	370-410	marine humic-like
P	398	660	pigment-like
T	275	340	tryptophan-like

When a range of wavelengths specified in one or both axes, the maximal signal value over that range is taken.
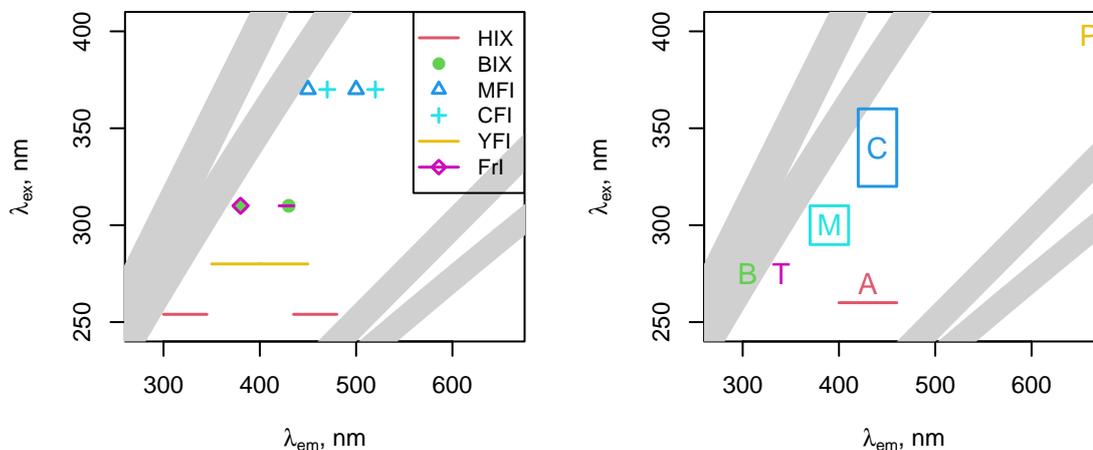
Positions of the peaks and the areas used to determine the fluorescence indices of an EEM. The Rayleigh and Raman scattering areas for both 1st and 2nd diffraction orders are shown in grey, assuming a width of ± 20 nm and a Raman shift of $3400\ \mathrm{cm}^{-1}$. The tolerance interval of ± 1 nm is invisible at the scale of the figure.

Integration for HIX and YFI is done using the trapezoidal method:

$$\int_a^b f(x)dx \approx (b-a)\frac{f(a)+f(b)}{2}$$

Value

For individual `feem` objects, a named numeric vector containing the values requested via the `indices` argument.

Otherwise, a `data.frame` containing the values from the vectors above and a column named `sample` containing the names of the samples (or numbers, if names were absent).

Author(s)

With edits and suggestions by Anastasia Drozdova.

References

Coble PG (2007). "Marine Optical Biogeochemistry: The Chemistry of Ocean Color." *Chemical Reviews*, **107**(2), 402-418. doi:10.1021/cr050350+.

Cory RM, McKnight DM (2005). "Fluorescence spectroscopy reveals ubiquitous presence of oxidized and reduced quinones in dissolved organic matter." *Environmental science & technology*, **39**(21), 8142-8149. doi:10.1021/es0506962.

Heo J, Yoon Y, Kim D, Lee H, Lee D, Her N (2016). "A new fluorescence index with a fluorescence excitation-emission matrix for dissolved organic matter (DOM) characterization." *Desalination and Water Treatment*, **57**(43), 20270-20282. doi:10.1080/19443994.2015.1110719.

Huguet A, Vacher L, Relexans S, Saubusse S, Froidefond JM, Parlanti E (2009). "Properties of fluorescent dissolved organic matter in the Gironde Estuary." *Organic Geochemistry*, **40**(6), 706-719. doi:10.1016/j.orggeochem.2009.03.002.

McKnight DM, Boyer EW, Westerhoff PK, Doran PT, Kulbe T, Andersen DT (2001). "Spectrofluorometric characterization of dissolved organic matter for indication of precursor organic material and aromaticity." *Limnology and Oceanography*, **46**(1), 38-48. doi:10.4319/lo.2001.46.1.0038.

Wilson HF, Xenopoulos MA (2009). "Effects of agricultural land use on the composition of fluvial dissolved organic matter." *Nature Geoscience*, **2**(1), 37-41. doi:10.1038/ngeo391.

Zsolnay A, Baigar E, Jimenez M, Steinweg B, Saccomandi F (1999). "Differentiating with fluorescence spectroscopy the sources of dissolved organic matter in soils subjected to drying." *Chemosphere*, **38**(1), 45-50. doi:10.1016/S00456535(98)001660.

See Also

feem

Examples

```
data(feems)

x <- feemscatter(feems$a, rep(25, 4), 'omit')
feemindex(x)
feemindex(x, interpolate = 'whittaker')

feemindex(feems[2:3])
feemindex(feemcube(feems[4:5], TRUE))
```

---

feemjackknife   *Jack-knife outlier detection in PARAFAC models*

Description

Perform leave-one-out fitting + validation of PARAFAC models on a given FEEM cube.

Usage

```
feemjackknife(cube, ..., progress = TRUE)
## S3 method for class 'feemjackknife'
plot(
    x, kind = c('estimations', 'RIP', 'IMP'), ...
  )
## S3 method for class 'feemjackknife'
coef(
    object, kind = c('estimations', 'RIP', 'IMP'), ...
  )
```

Arguments

cube	A `feemcube` object.
progress	Set to FALSE to disable the progress bar.
x, object	An object returned by `feemjackknife`.
kind	Chooses what to plot (when called as plot(...)) or return as a `data.frame` (when called as coef(...)):

> **estimations** Produce the loadings from every leave-one-out model.
>
> **RIP** Produce a Resample Influence Plot, i.e. mean squared difference between loadings in overall and leave-one-out models plotted against mean squared residuals in leave-one-out models.
>
> **IMP** Produce an Identity Match Plot, i.e. scores in leave-one-out models plotted against scores in the overall model.

...	**feemjackknife** Passed as-is to `feemparafac` and, eventually, to **multiway** function `parafac`.

> **plot.feemjackknife** When kind is "RIP" or "IMP", pass a q argument to specify the quantile of residual values (for RIP) or absolute score differences (IMP) above which sample names (or numbers) should be plotted. Default value for q is 0.9.
>
> Remaining arguments are passed as-is to `xyplot`.
>
> **coef.feemjackknife** No further parameters are allowed.

Details

The function takes each sample out of the dataset, fits a PARAFAC model without it, then fits the outstanding sample to the model with emission and excitation factors fixed:

$$\hat{\mathbf{c}} = (\mathbf{A} * \mathbf{B})^+ \times \text{vec}(\mathbf{X})$$

The individual leave-one-out models (fitted loadings $\mathbf{A}$, $\mathbf{B}$ and scores $\mathbf{C}$) are reordered according to best Tucker's congruence coefficient match and rescaled by minimising $||\mathbf{A}\,\text{diag}(\mathbf{s}_\text{A}) - \mathbf{A}^{\text{orig}}||^2$ and $||\mathbf{B}\,\text{diag}(\mathbf{s}_\text{B}) - \mathbf{B}^{\text{orig}}||^2$ over $\mathbf{s}_\text{A}$ and $\mathbf{s}_\text{B}$, subject to $\text{diag}(\mathbf{s}_\text{A}) \times \text{diag}(\mathbf{s}_\text{B}) \times \text{diag}(\mathbf{s}_\text{C}) = \mathbf{I}$, to make them comparable.

Once the models are fitted, resample influence plots and identity match plots can be produced from resulting data to detect outliers.

To conserve memory, feemjackknife puts the user-provided cube in an environment and passes it via envir and subset options of `feemparafac`. This means that, unlike in `feemparafac`, the cube argument has to be a `feemcube` object and passing envir and subset options to feemjackknife is not supported. It is recommended to fully name the parameters to be passed to `feemparafac` to avoid problems.

`plot.feemjackknife` provides sane defaults for `xyplot` parameters xlab, ylab, scales, as.table, but they can be overridden.

Value

feemjackknife A list of class feemjackknife containing the following entries:

> **overall** Result of fitting the overall cube with `feemparafac`.
>
> **leaveone** A list of length dim(cube)[3] containing the reduced dataset components. Every `feemparafac` object in the list has an additional Chat attribute containing the result of fitting the excluded spectrum back to the loadings of the reduced model.

plot.feemjackknife A **lattice** plot object. Its `print` or `plot` method will draw the plot on an appropriate plotting device.

coef.feemjackknife A `data.frame` containing various columns, depending on the value of the `kind` argument:

    estimations loading Values of the loadings.

        mode The axis of the loadings, "Emission" or "Excitation".

        wavelength Emission or excitation wavelength the loading values correspond to.

        factor The component number.

        omitted The sample (name if cube had names, integer if it didn't) that was omitted to get the resulting loading values.

    RIP msq.resid Mean squared residual value for the model with a given sample omitted.

        Emission Mean squared difference in emission mode loadings between the overall model and the model with a given sample omitted.

        Excitation Mean squared difference in excitation mode loadings between the overall model and the model with a given sample omitted.

        omitted The sample (name if cube had names, integer if it didn't) that was omitted from a given model.

    IMP score.overall Score values for the overall model.

        score.predicted Score values estimated from the loadings of the model missing a given sample.

        factor The component number.

        omitted The sample (name if cube had names, integer if it didn't) that was omitted from a given model.

References

Riu J, Bro R (2003). "Jack-knife technique for outlier detection and estimation of standard errors in PARAFAC models." *Chemometrics and Intelligent Laboratory Systems*, **65**(1), 35-49. doi:10.1016/S01697439(02)000904.

See Also

feemparafac, feemcube

Examples

```
data(feems)
cube <- feemscale(feemscatter(cube, rep(14, 4)), na.rm = TRUE)
# takes a long time
jk <- feemjackknife(cube, nfac = 3)
# feemparafac methods should be able to use the environment and subset
plot(jk$leaveone[[1]])
plot(jk)
plot(jk, 'IMP')
plot(jk, 'RIP')
head(coef(jk))
```

feemlist	*Create lists of FEEM objects*

Description

Convert vectors of file names or objects from other packages (such as **eemR** or **EEM**) into flat named lists of feem objects.

Usage

```
  feemlist(x, ...)
  ## S3 method for class 'character'
feemlist(
    x, format, pattern = NULL, recursive = TRUE, ignore.case = FALSE,
    simplify.names = TRUE, ...
  )
  ## S3 method for class 'eemlist'
feemlist(x, ...)
  ## S3 method for class 'EEM'
feemlist(x, ...)
```

Arguments

x	A character vector containing names of files and directories to import using feem.
	Alternatively, an eemlist object from the **eemR** package or an EEM object from the **EEM** package.
format	Corresponds to the format argument of feem. Currently, one format is assumed for all files to be imported.
	Alternatively, can be a function that takes a path to a file and anything passed in ... and returns a feem object corresponding to the file. This is done to make it easier to import groups of files in formats not yet supported by feem itself.
pattern, recursive, ignore.case	
	These options are passed to list.files for directories encountered in x and can be used to e.g. only choose files with a given suffix in the name. Note the non-default value for the recursive option.
simplify.names	If TRUE (default), split resulting names by the path separator (/, also \ on Windows) and remove leading components that have the same value for all samples, but leave at least one component. See Details on how this is related to name generation.
...	When importing files, remaining options are passed to feem or the import function passed in the format argument. Otherwise, no options are allowed.

Details

Names of x are preserved; if x is not named, names are assigned from the values of x itself, and so are empty names in partially-named x. Every directory in x is replaced with its contents (as returned by list.files), their names obtained by concatenating the name of the directory element with their paths inside the directory (with .Platform$file.sep as a separator). For example, when

importing x = c('foo' = 'bar') with directory 'bar' containing 'baz.txt', resulting name would be 'foo/baz.txt'.

When importing many files from the same directory, the simplify.names option is useful to avoid duplication in resulting names. For example, feemlist('.', simplify.names = FALSE) results in a list with all names starting with ./, while feemlist('foo/bar/baz', simplify.names = TRUE) (default) would shave off all three common path components and the separators.

Mixing files and directories in x will most likely not preserve the order of the elements.

Note: Please don't rely on the name generation behaving exactly as specified as it may be changed in the future versions.

When importing custom file formats, the format function should typically take the following form:

```
function(filename, ...) {
  # read data from filename
  # take additional arguments passed from feemlist(...) if needed
  return(feem(data))
}
```

Value

A flat named list of [feem](#) objects.

See Also

[feem](#); the packages **eemR** and **EEM**.

Examples

```
feemlist(
  system.file('extdata/pano2.txt', package = 'albatross'),
  'table', transpose = TRUE, na = 0
)
if (requireNamespace('eemR')) feemlist(eemR::eem_read(
  system.file('extdata/ho_aq.csv', package = 'albatross'),
  import_function='aqualog'
))
if (requireNamespace('EEM')) feemlist(EEM::readEEM(
  system.file('extdata/ho_aq.dat', package = 'albatross')
))
feemlist(
  system.file('extdata/custom.rds', package = 'albatross'),
  readRDS
)
```

---

feemparafac   *Compute PARAFAC on a FEEM cube object and access the results*

Description

feemparafac forwards its arguments to [parafac](#) from the **multiway** package, optionally rescales the result and attaches a few attributes. Resulting objects of class feemparafac can be accessed using methods presented below.

Usage

```
  feemparafac(
    X, ..., const = rep('nonneg', 3),
    rescale = 3, retries = 10, subset = TRUE, envir = NULL
  )
  ## S3 method for class 'feemparafac'
plot(x, type = c("image", "lines"), ...)
  ## S3 method for class 'feemparafac'
coef(
    object, type = c(
      "all", "scores", "loadings", "emission", "excitation", "samples"
    ), ...
  )
  ## S3 method for class 'feemparafac'
fitted(object, ...)
  ## S3 method for class 'feemparafac'
residuals(object, ...)
  ## S3 method for class 'feemparafac'
reorder(x, neworder, like, ...)
  ## S3 method for class 'feemparafac'
rescale(x, mode, newscale, absorb, like, ...)
```

Arguments

X	A FEEM cube object. The per-sample factors will be multiplied by attr(X, 'scales') stored in it.
	If envir is NULL (by default), this should be just a value. If envir is given, this should be a name of the value to get from the environment.
...	**feemparafac** Passed as-is to parafac.
	plot.feemparafac Passed as-is to **lattice** functions levelplot and xyplot.
	reorder.feemparafac, rescale.feemparafac Forwarded to the respective **multiway** functions.
	coef.feemparafac, fitted.feemparafac, residuals.feemparafac No other parameters are allowed.
const	A character vector of length 3 specifying the constraints for all modes of X, passed to parafac. Defaults to non-negativity. See const for more information.
rescale	Rescale the resulting factors to leave all the variance in the given mode: emission, excitation, or sample (default). Set to NA to disable.
retries	Retry for given number of tries until parafac returns a successfully fitted model or stops due to the iteration number limit. Raise a fatal error if all tries were unsuccessful.
subset	An integer or logical vector choosing the samples from X, as in feemparafac(X[, ,subset], ...). Defaults to the whole cube.
envir	An environment to look up X in.
x, object	An object returned by feemparafac.
type	Given a fitted PARAFAC model:

$$X_{i,j,k} = \sum_r A_{i,r} B_{j,r} C_{k,r}$$

With **A** corresponding to fluorescence emission loadings, **B** corresponding to fluorescence excitation loadings, and **C** corresponding to the scores of the components in different samples, the following plots can be produced:

image Plot the factors ("loadings") as a series of pseudo-colour images of outer products $\mathbf{a}_r \times \mathbf{b}_r^\top$

lines Plot the factors $\mathbf{a}_r$ and $\mathbf{b}_r$ as functions of wavelengths, with each pair of factors on a different panel.

Fitted PARAFAC coefficients can be returned in the following forms:

emission, excitation, samples Return the contents of **A**, **B** or **C**, respectively, as a [data.frame](#) with three columns, the first one (named `wavelength` or `sample`) containing the independent variable (λ_em / λ_ex / sample name or number), the second one (named `value`) containing the values and the third one (named `factor`) containing the factor numbers.

scores Same as samples.

loadings Same as "emission" and "excitation" combined using [rbind](#), with a fourth column (`mode`) added, naming the kinds of loadings.

all A list with names "emission", "excitation", "samples" containing results of `coef(object, "emission")`, `coef(object, "excitation")`, `coef(object, "samples")`, respectively.

neworder   A permutation of integers between 1 and `ncol(x$A)` (the number of components) specifying the new order of factors. Forwarded to [reorder.parafac](#). Incompatible with the `like` argument.

like   A `feemparafac` object.

In `reorder`, the factors in `x` will be reordered to match the factors in `like` according to the smallest of the cosine similarities ([congru](#)) for the emission and excitation wavelengths.

In `rescale`, every factor matrix **A** from `x` that was specified in `mode` will be multiplied by scaling factors **c** so in order to minimise $\|\mathbf{A}_\texttt{like} - \text{diag}(\mathbf{c})\mathbf{A}_\mathbf{x}\|^2$.

mode   The modes to rescale, with `"A"`, `"B"`, `"C"` corresponding to emission, excitation, and samples, respectively. When `like` is specified, defaults to `c("A", "B")`. Forwarded to [rescale.parafac](#).

newscale   The desired root-mean-square for each column of the modes being rescaled. Forwarded to [rescale.parafac](#). Incompatible with the `like` argument.

absorb   The mode that should absorb the inverse rescaling coefficients. When `like` is specified, defaults to `"C"`. Forwarded to [rescale.parafac](#).

Details

feemparafac tries hard to guarantee the convergence flag to be 0 (normal convergence) or 1 (iteration number limit reached), but never 2 (a problem with the constraints). A fatal error is raised if repeated runs of [parafac](#) do not return a (semi-)successfully fitted model.

After the PARAFAC decomposition is calculated, the scores are multiplied by the scales attribute of the X object, making them represent the cube with scaling undone. Use [feemscale](#)(remember = FALSE) if you don't want to undo the scaling.

The output option is fixed to `"best"` value. Obtaining a list of alternative solutions can therefore be achieved by running:

```
replicate(n, feemparafac(..., nstart = 1), simplify = FALSE)
```

The subset and envir options are useful to repeatedly perform PARAFAC on different subsets of the same FEEM cube, e.g. in jack-knifing or split-half analysis. Since feemparafac keeps a

reference to the its X and envir arguments, the use of subset should ensure that the same FEEM cube is referenced from multiple feemparafac objects instead of creating copies of its subsets. Additionally, environment objects are not duplicated on [save](#) or [load](#), so storing X in an environment and passing it to multiple invocations of feemparafac will save a lot of memory when the results are serialised together.

plot.feemparafac provides sane defaults for **lattice** options such as xlab, ylab, as.table, auto.key, type, cuts, col.regions, but they can be overridden.

Value

feemparafac   An object of classes feemparafac and parafac with the following attributes added:

> **cube** A copy of the X argument.
>
> **subset** A copy of the subset argument.
>
> **envir** A copy of the envir argument.
>
> [rownames](#) are added from the original data cube to the A, B, C components of the list returned by [parafac](#).
>
> Use [feemcube](#) on the return value to access the original data cube.

plot.feemparafac

> A **lattice** plot object. Its print or plot method will draw the plot on an appropriate plotting device.

coef.feemparafac

> A [data.frame](#) or a list of them (only if type is "all"). See the description of the type argument for more information.

fitted.feemparafac

> A [feemcube](#) object comparable to X as it was decomposed by [parafac](#), ignoring the scaling.

resid.feemparafac

> A [feemcube](#) object equal to $\mathbf{X} - \hat{\mathbf{X}}$, with an additional class feem.resid set. Objects of this class are plotted with a different default palette, see [plot.feem.resid](#).

References

Bro R (1997). "PARAFAC. Tutorial and applications." *Chemometrics and Intelligent Laboratory Systems*, **38**(2), 149-171. [doi:10.1016/S01697439(97)000324](#).

See Also

[parafac](#) class structure; [write.openfluor](#), [feemcube](#) for methods specific to values returned from this function.

Examples

```
data(feems)
cube <- feemscale(feemscatter(cube, rep(14, 4)), na.rm = TRUE)
(factors <- feemparafac(cube, nfac = 3))
plot(factors, 'image')
plot(factors, 'line')
head(coef(factors, 'loadings'))
str(coef(factors, 'all'))
str(feemcube(factors)) # original cube is retained
plot(fitted(factors))
plot(resid(factors))
```

---

feems *Synthetic fluorescence excitation-emission matrices and absorbance spectra*

Description

This dataset consists of twelve fluorescence and absorbance spectra simulated from three trilinear components, with scattering signal added and divided by a correction factor to simulate inner filter effect.

Usage

```
data("feems")
```

Format

feems A named list of 12 feem objects containing fluorescence data measured with excitation wavelengths between 230 nm and 350 nm (with a step of 2 nm) and emission wavelengths between 240 nm and 435 (with a step of 5 nm).

cube A 12-sample feemcube object consisting of of 32 by 10 FEEMs measured at the same wavelength range as above with inner filter effect corrected.

absorp A 12-element named list containing absorbance spectra measured between 230 and 450 nm in 1 cm cells. Each element of the list is a two-column matrix. The first column contains the wavelengths and the second column contains the absorbance values.

Examples

```
data(feems)
plot(cube)
plot(feems$a)
matplot(
  absorp[[1]][,1],
  sapply(absorp, function(x) x[,2]),
  type = 'l', lty = 1
)
```

---

feemscale *Rescale FEEM spectra to a given norm and remember the scale factor*

Description

Given a norm function (typically, standard deviation), scale the intensities in FEEM objects to it and optionally remember the scale factor.

Usage

```
  feemscale(x, ...)
  ## S3 method for class 'feem'
feemscale(x, norm = sd, remember = TRUE, ...)
  ## S3 method for class 'feemcube'
feemscale(x, ..., progress = FALSE)
  ## S3 method for class 'list'
feemscale(x, ..., progress = FALSE)
```

Arguments

x	A FEEM object, a FEEM cube object, or a list of anything compatible with feemscale generic.
norm	A function taking a numeric matrix and returning its norm. Typically, sd or sumsq.
remember	Whether to remember the scale factor. If FALSE, the scale factor in the returned object is unchanged.
...	Passed as-is to feemscale, to feemscale.feem, then to the norm function. Use this to set na.rm = TRUE for functions like sd or sumsq.
progress	Set to TRUE to enable a progress bar (implemented via txtProgressBar).

Value

feemscale.feem: a FEEM object with intensities divided by scale factor (norm(x)) and its scale attribute multiplied by the scale factor.

feemscale.feemcube: a FEEM cube built from FEEM objects scaled as described above.

feemscale.list: a list consisting of results of feemscale generic applied to its elements.

References

Bro R, Smilde AK (2003). "Centering and scaling in component analysis." *Journal of Chemometrics*, **17**(1), 16-33. doi:10.1002/cem.773.

See Also

feem

Examples

```
feemscale(feem(matrix(1:42, 6), 1:6, 1:7))
```

| feemscatter | *Handle scattering signal in FEEMs* |

Description

Remove or interpolate scattering signal in individual FEEM objects, FEEM cube objects, or lists of them.

Usage

```
    feemscatter(x, ...)
    ## S3 method for class 'list'
feemscatter(x, ..., cl, progress = TRUE)
    ## S3 method for class 'feemcube'
feemscatter(x, ..., cl, progress = TRUE)
    ## S3 method for class 'feem'
feemscatter(
    x, widths, method = c("omit", "pchip", "loess", "kriging", "whittaker"),
    add.zeroes = 30, Raman.shift = 3400, ...
)
```

Arguments

x   An individual FEEM object, FEEM cube object, or a list of them, to handle the
                scattering signal in.

widths   A numeric vector or a list containing the half-widths of the scattering bands, in
                nm. Rayleigh scattering is followed by Raman scattering, followed by second
                diffraction order for Rayleigh and Raman, and so on. (Typically, there's no need
                for anything higher than third order, and even that is rare.) For example:

                1. Rayleigh scattering
                2. Raman scattering
                3. Rayleigh scattering, 2λ
                4. Raman scattering, 2λ
                5. ...

                For higher diffraction orders, the peak widths are proportionally scaled, mak-
                ing it possible to provide the same number for all kinds of scattering visible in
                the EEM. Set a width to 0 if you don't want to handle this particular kind of
                scattering signal.

                It's possible to specify the bands asymmetrically. If the area to be corrected
                should range from x nm to the left of the scattering peak to y nm to the right
                of it, pass a list instead of a vector, and put a two-element vector c(x, y) for
                the appropriate kind of scattering. For example, passing widths = list(c(30,
                20), 20) means "handle -30 nm to the left and $+20$ nm to the right of Rayleigh
                peak and ± 20 nm around Raman peak".

                To sum up, given two half-widths W_1 and W_2, the test for being inside a kth
                diffraction order of a scattering band is as follows:

                $$-W_1 < \frac{\lambda_{\text{center}}}{k} - \lambda_{\text{em}} < +W_2$$

widths = list(c(50, 20), 20, 20, 20, 10), Raman.shift = 3400
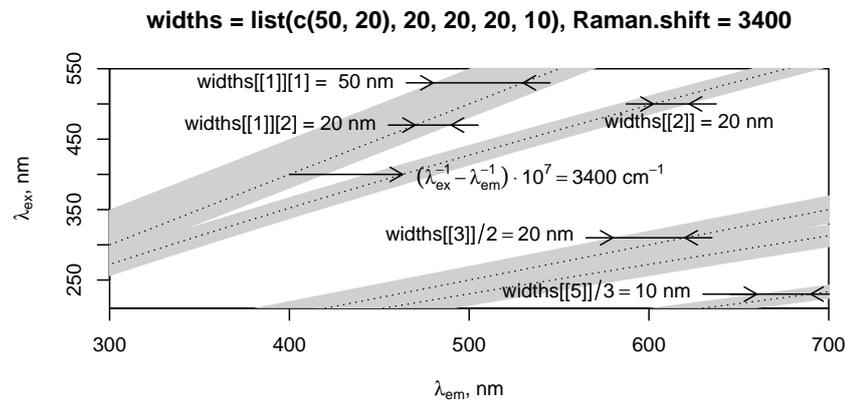
In this example, a much larger portion of the anti-Stokes area is removed near the first order Rayleigh scattering signal than in the Stokes area. This can be useful to get rid of undesired signal where no fluorescence is observed on some spectrometers. The second and third order scattering signal areas are automatically scaled 2 and 3 times, respectively.

method   A string choosing *how* to handle the scattering signal:

omit Replace it with NA.

pchip Interpolate it line-by-line using piecewise cubic Hermitean polynomials (`pchip`). Pass a by argument to choose the direction of interpolation; see Details.

loess Interpolate it by fitting a locally weighted polynomial surface (`loess`). Extra arguments are passed verbatim to `loess`, which may be used to set parameters such as span.

kriging Interpolate it by means of ordinary or simple Kriging, as implemented in **pracma** function `kriging`. Pass a type argument to choose between the two methods. This method is not recommended due to its high CPU time and memory demands: it has to invert a dense $O(N^2)$ matrix (which easily reaches multiple gigabytes for some EEMs), and compute its product with a vector then take scalar products $O(N)$ times, with $N = \texttt{length(x)}$.

whittaker Interpolate it by minimising a weighted sum of squared residuals (for known part of the spectrum) and roughness penalty (squared central difference approximations for derivatives by λ_{em} and λ_{ex}). See Details for more information and parameters.

add.zeroes   Set intensities at $\lambda_{em} < \lambda_{ex} - \texttt{add.zeroes}$ nm to 0 unless they have been measured in order to stabilise the resulting decomposition (Thygesen, Rinnan, Barsberg, and Møller 2004). Set to NA to disable this behaviour.

Raman.shift   Raman shift of the scattering signal of water, cm^{-1}.

...   Passed verbatim from feemscatter generics to feemscatter.feem.

If "pchip" method is selected, the by parameter chooses between interpolating by row, by column, or averaging both, see Details.

If "loess" method is selected, remaining options are passed to `loess` (the span parameter is of particular interest there).

If "kriging" method is selected, remaining options are passed to `kriging`.

If "whittaker" method is selected, available parameters include d, lambda, nonneg and logscale, see Details.

cl   If not missing, a **parallel** cluster object to run the scattering correction code on
                    or NULL for the default cluster object registered via setDefaultCluster.

progress   Set to FALSE to disable the progress bar.

Details

The "pchip" method works by default as described in (Bahram, Bro, Stedmon, and Afkhami 2006):
each emission spectrum at different excitation wavelengths is considered one by one. Zeroes are
inserted in the corners of the spectrum if they are undefined (NA) to prevent extrapolation from
blowing up, then the margins are interpolated using the corner points, then the rest of the spectrum
is interpolated line by line. Since pchip requires at least 3 points to interpolate, the function falls
back to linear interpolation if it has only two defined points to work with. The by argument controls
whether the function proceeds by rows of the matrix ("emission", default), by columns of the matrix
("excitation"), or does both ("both") and averages the results to make the resulting artefacts less
severe (Pucher, Wünsch, Weigelhofer, Murphy, Hein, and Graeber 2019) (see the **staRdom** package
itself).

The "loess" method feeds the whole FEEM except the area to be interpolated to loess, then asks it
to predict the remaining part of the spectrum. Any negative values predicted by loess are replaced
by 0.

The "kriging" method (Press, Teukolsky, Vetterling, and Flannery 2007) is much more computa-
tionally expensive than the previous two, but, on some spectra, provides best results, not affected
by artefacts resulting from line-by-line one-dimensional interpolation (pchip) or varying degrees
of smoothness in different areas of the spectrum (loess). Any negative values returned by kriging
are replaced by 0.

> **Whittaker smoothing:**   The "whittaker" method (Krylov and Labutin 2023) works by minimis-
> ing a sum of penalties, requiring the interpolated surface to be close to the original points around
> it and to be smooth in terms of derivatives by λ_{em} and λ_{ex}.
>
> The parameters d and lambda should be numeric vectors of the same length, corresponding to the
> derivative orders (whole numbers ≥ 1) and their respective penalty weights (small real numbers;
> larger is smoother). For interpolation purposes, the default penalty is $10^{-2}\mathbf{D}_1 + 10\mathbf{D}_2$, which
> corresponds to d = 1:2 and lambda = c(1e-2, 10).
>
> Any resulting negative values are pulled towards 0 by adding zero-valued points with weight
> nonneg (default 1) and retrying. Set nonneg to 0 to disable this behaviour. It is also possible to
> deal with resulting negative values by scaling and shifting the signal between logscale (typically)
> and 1, interpolating the logarithm of the signal, then undoing the transformation. By default
> logscale is NA, disabling this behaviour, since it may negatively affect the shape of interpolated
> signal.
>
> See the internal help page whittaker2 for implementation details.

Value

An object of the same kind (FEEM object / FEEM cube / list of them) with scattering signal handled
as requested.

References

Bahram M, Bro R, Stedmon C, Afkhami A (2006). "Handling of Rayleigh and Raman scatter for
PARAFAC modeling of fluorescence data using interpolation." *Journal of Chemometrics*, **20**(3-4),
99-105. doi:10.1002/cem.978.

Krylov IN, Labutin TA (2023). "Recovering fluorescence spectra hidden by scattering signal: in search of the best smoother." *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 122441. doi:10.1016/j.saa.2023.122441.

Press WH, Teukolsky SA, Vetterling WT, Flannery BP (2007). "Interpolation by Kriging." In *Numerical recipes: The Art of Scientific Computing (3rd Ed.)*, chapter 3.7.4, 144-147. Cambridge University Press, New York.

Pucher M, Wünsch U, Weigelhofer G, Murphy K, Hein T, Graeber D (2019). "staRdom: Versatile Software for Analyzing Spectroscopic Data of Dissolved Organic Matter in R." *Water*, **11**(11), 2366. doi:10.3390/w11112366.

Thygesen LG, Rinnan Å, Barsberg S, Møller JKS (2004). "Stabilizing the PARAFAC decomposition of fluorescence spectra by insertion of zeros outside the data area." *Chemometrics and Intelligent Laboratory Systems*, **71**(2), 97-106. ISSN 0169-7439, doi:10.1016/j.chemolab.2003.12.012.

See Also

feem, feemcube

Examples

```
data(feems)
plot(x <- feemscatter(
  feems[[1]], widths = c(25, 25, 20, 20),
  method = 'whittaker', Raman.shift = 3500
))
```

---

feemsplithalf	*Split-half analysis of PARAFAC models*

Description

This function validates PARAFAC with different numbers of components by means of splitting the data cube in halves, fitting PARAFAC to them and comparing the results (DeSarbo 1984).

Usage

```
feemsplithalf(
  cube, nfac, splits, random, groups, fixed, ..., progress = TRUE
)
## S3 method for class 'feemsplithalf'
plot(x, kind = c('tcc', 'factors'), ...)
## S3 method for class 'feemsplithalf'
print(x, ...)
## S3 method for class 'feemsplithalf'
coef(object, kind = c('tcc', 'factors'), ...)
```

Arguments

cube	A feemcube object.
nfac	An integer vector of numbers of factors to check.

splits   A scalar or a two-element vector consisting of whole numbers.

                The first element is the number of parts to split the data cube into, which must
                be even. After splitting, the parts are recombined into non-intersecting halves
                (Murphy, Stedmon, Graeber, and Bro 2013), which are subjected to PARAFAC
                decomposition and compared against each other.

                The second element, if specified, limits the total number of comparisons be-
                tween the pairs, since the number of potential ways to recombine the parts of
                the data cube into halves grows very quickly.

                The number of PARAFAC models fitted is $2 \cdot$ splits[2]. If only splits[1] is
                specified, splits[2] defaults to $\binom{\text{splits}[1]}{\text{splits}[1]/2}$.

                Mutually incompatible with the parameters random, fixed.

random   Number of times to shuffle the dataset, split into non-intersecting halves, fit a
                PARAFAC model to each of the halves and compare halves against each other
                (Krylov, Drozdova, and Labutin 2020).

                The number of PARAFAC models fitted is $2 \cdot$ random.

                Mutually incompatible with the parameters splits, fixed.

groups   Use this argument to preserve the ratios between the groups present in the orig-
                inal dataset when constructing the halves. If specified, must be a factor or an
                integer vector of length dim(cube)[3] (specifying the group each sample be-
                longs to) or a list of them, i.e., a valid f argument to [split](). By default, samples
                are considered to form a single group.

                For the split-combine method (splits), each group must have at least splits
                elements; for best results, sizes of groups should be close to a multiple of
                splits. For the randomised split-half method (random), each group should
                have at least 2 elements.

                Mutually incompatible with the fixed parameter.

fixed   Use this argument to manually specify the contents of the halves to test. The
                argument must be a list containing two-element lists specifying the halves to
                compare. Each half must be a vector consisting of whole numbers specifying
                sample indices in the cube (see the example).

                It is considered an error to specify a sample in both halves.

                Mutually incompatible with the parameters splits, random, groups.

progress   Set to FALSE to disable the progress bar.

x, object   An object returned by feemsplithalf.

kind   Chooses what type of data to return or plot:

                tcc Statistics of between-half TCCs for different numbers of components. The
                    smallest TCC is chosen between emission- and excitation-mode values, but
                    otherwise they are not aggregated.
                    When plotting, TCC values for the component with the same number have
                    the same colour.

                factors The resulting loading values.
                    When plotting, split the plot into panels per each number of components
                    and each mode (emission or excitation). Components with the same number
                    have the same colour.

...   **feemsplithalf** Remaining options are passed to [feemparafac]() and, eventually,
                    to [parafac](). It is recommended to fully name the parameters instead of
                    relying on partial or positional matching.

                plot.feemsplithalf Passed as-is to [xyplot]().

                print.feemsplithalf, coef.feemsplithalf No additional options are allowed.

Details

As the models (loadings $\mathbf{A}$, $\mathbf{B}$ and scores $\mathbf{C}$) are fitted, they are compared to the first model of the same number of factors (Tucker's congruence coefficient is calculated using [congru](#) for emission and excitation mode factors, then the smallest value of the two is chosen for the purposes of matching). The models are first reordered according to the best match by TCC value, then rescaled (Riu and Bro 2003) by minimising $||\mathbf{A}\,\mathrm{diag}(\mathbf{s}_A) - \mathbf{A}^{\mathrm{orig}}||^2$ and $||\mathbf{B}\,\mathrm{diag}(\mathbf{s}_B) - \mathbf{B}^{\mathrm{orig}}||^2$ over $\mathbf{s}_A$ and $\mathbf{s}_B$, subject to $\mathrm{diag}(\mathbf{s}_A) \times \mathrm{diag}(\mathbf{s}_B) \times \mathrm{diag}(\mathbf{s}_C) = \mathbf{I}$, to make them comparable.

To perform stratified sampling on a real-valued variable (e.g. salinity, depth), consider binning samples into groups using [cut](#), perhaps after histogram flattening using `ecdf(x)(x)`. To determine the number of breaks, consider [nclass.Sturges](#).

To conserve memory, feemsplithalf puts the user-provided cube in an environment and passes it via envir and subset options of [feemparafac](#). This means that, unlike in [feemparafac](#), the cube argument has to be a [feemcube](#) object and passing envir and subset options to feemsplithalf is not supported.

plot.feemsplithalf plots results of the split-half procedure (TCC or loading values depending on the kind argument) using **lattice** graphics. Sane defaults are provided for [xyplot](#) parameters xlab, ylab, as.table, but they can be overridden.

print.feemsplithalf displays a very short summary of the analysis, currently the minimum TCC value for each number of components.

coef.feemsplithalf returns the Tucker's congruence coefficients resulting from the split-half analysis.

Value

feemsplithalf, print.feemsplithalf An object of class feemsplithalf, containing named fields:

> **factors** A [list](#) of [feemparafac](#) objects containing the factors of the halves. The list has dimensions, the first one corresponding to the halves (always 2), the second to different numbers of factors (as many as in nfac) and the third to different groupings of the samples (depends on splits or random).
>
> **tcc** A named list containing arrays of Tucker's congruence coefficients between the halves. Each entry in the list corresponds to an element in the nfac argument. The dimensions of each array in the list correspond to, in order: the factors (1 to nfac[i]), the modes (emission or excitation) and the groupings of the samples (depending on splits or random).
>
> **nfac** A copy of nfac argument.

plot.feemsplithalf A **lattice** plot object. Its print or plot method will draw the plot on an appropriate plotting device.

coef.feemsplithalf A [data.frame](#) containing various columns, depending on the value of the kind argument:

> **tcc factor** The factor (out of nfac) under consideration.
>
> > **tcc** Tucker's congruence coefficient between a pair of matching components. Out of two possible values (TCC between excitation loadings or emission loadings), the minimal one is chosen, because the same rule is used to find which components match when reordering them in a pair of models.
> >
> > **test** The sequence number for each pair of models in the split-half test, related to the third dimension of object$factors or object$tcc. May be used to group values for plotting or aggregation.
> >
> > **subset** Consists of two-element lists containing indices of the samples in each half of the original cube.

nfac The number of factors in the pair of models under consideration.

factors wavelength Emission and excitation wavelengths.

value The values of the loadings.

factor Number of the factor, 1 to `nfac`.

mode The mode the loading value belongs to, "Emission" or "Excitation".

nfac Total number of factors.

test Sequence number of a split-half test, indicating a given way to split the dataset in a group of splits with the same numbers of factors.

half Number of the half, 1 or 2.

subset For every row, this is an integer vector indicating the subset of the original data cube that the loadings have been obtained from.

References

DeSarbo WS (1984). "An Application of PARAFAC to a Small Sample Problem, Demonstrating Preprocessing, Orthogonality Constraints, and Split-Half Diagnostic Techniques (Appendix)." *Research Methods for Multimode Data Analysis*, 602-642. https://papers.ssrn.com/abstract=2783446.

Krylov I, Drozdova A, Labutin T (2020). "Albatross R package to study PARAFAC components of DOM fluorescence from mixing zones of arctic shelf seas." *Chemometrics and Intelligent Laboratory Systems*, **207**(104176). doi:10.1016/j.chemolab.2020.104176.

Murphy KR, Stedmon CA, Graeber D, Bro R (2013). "Fluorescence spectroscopy and multi-way techniques. PARAFAC." *Analytical Methods*, **5**, 6557-6566. doi:10.1039/c3ay41160e.

Riu J, Bro R (2003). "Jack-knife technique for outlier detection and estimation of standard errors in PARAFAC models." *Chemometrics and Intelligent Laboratory Systems*, **65**(1), 35-49. doi:10.1016/S01697439(02)000904.

See Also

feemparafac, parafac, congru, feemcube.

Examples

```
data(feems)
cube <- feemscale(feemscatter(cube, rep(14, 4)), na.rm = TRUE)

(sh <- feemsplithalf(
  cube, 1:4, splits = 4 # => S4C6T3
  # splits = c(4, 2) would be S4C4T2, and so on
  # the rest is passed to multiway::parafac;
  # setting ctol and maxit is recommended
))

# specifying fixed halves to compare as list of 2-element lists
fixed <- list(
  list(1:6, 7:12),
  list(seq(1, 11, 2), seq(2, 12, 2))
)
sh.f <- feemsplithalf(cube, 2:3, fixed = fixed)

# can use feemparafac methods for individual models in $factors
plot(sh$factors[[1]])
```

```
plot(sh)
plot(sh, 'factors')
head(coef(sh))
head(coef(sh, 'factors'))
```

---

marine.colours	*Perceptually uniform palettes*

Description

Create perceptually continuous palettes of R colours.

Usage

```
marine.colours(
  n, chroma = 0.65, luminance = c(0.35, 1),
  alpha = 1, gamma = 1, fixup = TRUE
)
diverging.colours(
  n, chroma = c(.1, .75), luminance = c(1, .35),
  alpha = 1, gamma = 1, fixup = TRUE
)
```

Arguments

n	Number of colours to return.
chroma	Specifies the chroma (how saturated should the colours be) for the palette, a real number between 0 and 1. May also be a two-element vector, in which case the chroma is changed smoothly from start to finish of the resulting palette.
luminance	Specifies the luminance (how bright should the colours be) of the colours constituting the palette. Typically, a two-element vector of real numbers between 0 and 1 to indicate smooth change along the palette, but can also be a fixed number.
alpha	Specifies the transparency of the colours of the palette. As above, can be a fixed number or a two-element vector in the range $[0, 1]$. Typically, fully opaque (alpha=1) colours are used.
gamma	Provides the power coefficient for the hue/chroma/luminance/alpha growth formulae. May be useful when it is needed to sacrifice the perceptual linearity of the palette to provide more contrast for smaller or bigger values on the plot. The gamma-corrected values are obtained by computing x^γ, $x \in [0; 1]$, then scaling the result linearly to the required range. Typically, linear growth (gamma = 1) is preferred.
fixup	Whether to correct the palette if the resulting colours happen to fall outside the valid RGB range (passed as-is to hcl). Unrepresentable colours are returned as NAs, but fixing the palette may make it less perceptually uniform.

Details

The `marine.colours` palette is used by default by all `plot` methods (e.g. `plot.feem`) for FEEM-like data to show absolute values. It is designed to retain perceptual uniformity even after complete desaturation.

The `diverging.colours` palette is used by `plot.feem.resid` to display residual values. People with severe colour vision deficiency (tritanopia or monochromacy) won't be able to discern positive and negative branches of the palette, but it's supposed to be legible for people with deuteranopia and protanopia.

Value

A character vector of length `n` containing colour specifications for use with R graphics functions.

The `marine.colours` palette at the default values of $C_{uv}^* = 0.65$, $L^* \in [0.35; 1]$, $\alpha = \gamma = 1$.

The `diverging.colours` palette at the default values of $C_{uv}^* \in [0.1; 0.75]$, $L^* \in [0.35; 1]$, $\alpha = \gamma = 1$.

References

Insired by cmocean palette called "haline" (https://matplotlib.org/cmocean/#haline), but using R's implementation of polar CIE-LUV colour space instead of CAM02-UCS.

CUBEHELIX (https://www.mrao.cam.ac.uk/~dag/CUBEHELIX/) is a similar technique using BT.601 luminance coefficients and RGB colour space.

See Also

`plot.feem`, `hcl`

Examples

```
image(volcano, col = marine.colours(256))
```

---

plot.feem   *Plot a FEEM object*

Description

Plot a 2D fluorescence intensity surface as a pseudo-colour image.

Usage

```
## S3 method for class 'feem'
plot(
  x,
  xlab = quote(lambda[em] * " , nm"), ylab = quote(lambda[ex] * " , nm"),
  cuts = 128, col.regions = marine.colours(256), ...
)
```

```
## S3 method for class 'feemcube'
plot(
  x,
  xlab = quote(lambda[em] * " , nm"), ylab = quote(lambda[ex] * " , nm"),
  cuts = 128, col.regions = marine.colours(256), as.table = TRUE, ...
)
## S3 method for class 'feem.resid'
plot(
  x, ..., at, col.regions = diverging.colours(256)
)
```

Arguments

x	An FEEM object.
xlab	The x-axis label for the plot, with a sane default.
ylab	The y-axis label for the plot, with a sane default.
cuts	The number of distinct levels the intensity would be divided into, areas between them assigned different colours.
col.regions	The palette to take the colours from, a character vector of R colour specifications.
at	The breakpoints in the intensity values. For residual plots, automatically set in a symmetric manner, ignoring the cuts argument.
as.table	Whether to draw the panels left to right, top to bottom. (Otherwise they are drawn left to right, bottom to top.)
...	Passed as-is to [levelplot]().

Value

A [lattice]() plot object. Its print or plot method will draw the plot on an appropriate plotting device.

See Also

[levelplot]()

Examples

```
plot(feem(matrix(1:42/42, nrow = 7), 320 + 1:7, 300 + 1:6))
```

---

write.openfluor   *Export a PARAFAC model for the OpenFluor database*

Description

Prepares a fitted PARAFAC model for submission to OpenFluor - an online spectral database of fluorescence by environmental organic compounds.

Usage

```
write.openfluor(
  model, filename, name = "?", creator = "?", doi = "?",
  reference = "?", unit = "?", toolbox =, date =, fluorometer = "?",
  constraints =, validation = "?", methods = "?", preprocess = "?",
  sources = "?", ecozones = "?", description = "",
  shift = FALSE, scale = TRUE
)
```

Arguments

`model`	A [feemparafac](#) object.
`filename`	Path to the text file to create from the `model` argument.
`name`	Short name of the model.
`creator`	Name of the creator of the model.
`doi`	Digital object identifier of the referenced source. Can also be "ISBN:..." for books.
`reference`	Full citation for the referenced source using the following style: "Author AA, Author BB, Author CC, (year), 'Title', Journal Abbrev, Vol, pages".
`unit`	Units the fluorescence was measured in. Typically, one of "RU", "QSE", "AU".
`toolbox`	Defaults to "albatross *version*, multiway *version*".
`date`	Defaults to today, in "*yyyy-mm-dd*" format.
`fluorometer`	The model of the instrument that produced the data.
`constraints`	Constraints applied to the PARAFAC model. Defaults to `model$const`, but please edit it to a more human-readable form.
`validation`	Validation method used for the PARAFAC model, examples include: "Split-Half Analysis", "core-consistency".
`methods`	The sequence of steps taken to handle the samples and to ensure proper fluorescence intensity measurement. Examples include:

- Sampling: Filtration GF/F
- Sampling: Filtration *x* um
- Sampling: samples frozen
- Instrument spectral bias correction: Ex
- Instrument spectral bias correction: Em
- Instrument spectral bias correction: Ex & Em
- Inner filter effect correction: absorbance method
- Inner filter effect correction: dilution
- Inner filter effect correction: CDA
- Inner filter effect correction: *other (please describe)*
- Internal calibration: Raman Peak area
- Internal calibration: Raman Peak height
- Internal calibration: Blank Subtraction
- External calibration: Quinine Sulphate dilution series
- External calibration: STARNA reference standards
- External calibration: NIST reference standards
- External calibration: *other (please describe)*

preprocess   PARAFAC-specific pre-processing steps applied to the dataset. Examples in-
                 clude (but are not limited to):

- Outliers removed
- Scatter region excised (replaced with NaNs)
- Scatter region smoothed (replaced with interpolated values)
- Sample mode normalised to DOC concentration
- Sample mode normalised to unit variance

sources   Should preferably include one or more of the following keywords:

- river
- stream
- lake
- wetland
- reservoir
- estuary
- ocean - coastal and shelf seas
- ocean - surface off-shore
- ocean - deep off-shore
- freshwater
- seawater
- groundwater
- wastewater
- drinking water
- treated water
- recycled water
- ballast water
- sediment
- mudflat
- mangrove
- aquarium
- mesocosm

ecozones   List all major or minor terrestrial, freshwater and marine ecozones and ecore-
                 gions that apply. The full set of possible options is too large to include here, but
                 see https://en.wikipedia.org/wiki/Lists_of_ecoregions for a source of
                 inspiration.

description   Brief description of the model and its source data in ≤ 256 characters.

shift, scale   If shift is specified (default FALSE), the loadings are first shifted by subtracting
                 min(x) to ensure that the minimal value is 0.

                 If scale is specified (default TRUE), the loadings are then rescaled by dividing
                 by max(x) so that the maximal value is 1.

                 Note that OpenFluor clamps values outside the $[0, 1]$ range and uses scale-
                 invariant (but *not* shift-invariant) Tucker's congruence coefficient to find matches.

Details

Provided the model and the filename arguments, this function exports the loadings into a file that
passes OpenFluor syntax check and is suitable for further editing. Alternatively, some or all of the
fields may be specified programmatically.

The fields constraints, methods, preprocess, sources, ecozones can be specified as character
vectors (to be comma-separated on output); others should be single strings.

References

Murphy KR, Stedmon CA, Wenig P, Bro R (2014). "OpenFluor - an online spectral library of auto-fluorescence by organic compounds in the environment." *Analytical Methods*, **6**, 658-661. doi:10.1039/C3AY41935E.

https://openfluor.lablicate.com/

See Also

feemparafac

Examples

```
data(feems)
cube <- feemscale(feemscatter(cube, rep(14, 4)), na.rm = TRUE)
factors <- feemparafac(cube, nfac = 3)
# all defaults
write.openfluor(factors, f1 <- tempfile(fileext = '.txt'))
if (interactive()) file.show(f1)
unlink(f1)
# all non-default arguments
write.openfluor(
  factors, f2 <- tempfile(fileext = '.txt'), name = 'example',
  creator = 'J. Doe', doi = '10.1000/1', reference = paste(
    'Upper D, (1973),', "'The unsuccessful self-treatment of a case",
    "of \"writer's block\"',", 'J Appl Behav Anal, 7(3), 497'
  ), unit = 'AU', toolbox = 'all calculations done by hand',
  date = '2038-01-19', fluorometer = 'Acme Fluor-o-matic 9000',
  constraints = 'non-negative', validation = 'prior knowledge',
  methods = 'Instrument spectral bias correction: Ex & Em',
  preprocess = 'Scatter region excised (replaced with NaNs)',
  sources = 'freshwater', ecozones = 'Balkash',
  description = 'not a real model', shift = FALSE, scale = TRUE
)
if (interactive()) file.show(f2)
unlink(f2)
```

[.feem   *Extract or replace parts of FEEM objects*

Description

Extract or replace parts of FEEM spectra. Returns FEEM objects unless dimensions should be dropped. When assigning from a FEEM object, requires wavelengths to match and warns if scale factors differ.

Usage

```
  ## S3 method for class 'feem'
x[i, j, drop = TRUE]
  ## S3 replacement method for class 'feem'
x[i, j] <- value
```

Arguments

x	A FEEM object.
i, j	Row and column indices, respectively. As in usual R subsetting (see [Extract](#)), may be integer, logical or character vectors, or missing.
drop	Coerce result to the lowest possible dimension (dropping the feem class if so).
value	An array-like object to assign values from. When assigning from FEEM objects, wavelengths are required to match and warnings are issued if scale factors don't match. Use vector subsetting (zero or one argument inside the brackets) to disable the check.

Value

For [: If drop is TRUE and at least one of the index arguments chooses only one element along its axis, a named numeric vector. Otherwise, a FEEM object.

For [<-: a FEEM object.

See Also

feem, [.feemcube

Examples

```
(z <- feem(matrix(1:40, ncol = 8), 66 + 1:5, 99 + 1:8, 3))
str(z[1:4, 1:2])
str(z[1,, drop = TRUE])
z[2:3, 4:5] <- feem(matrix(1:4, 2), 66 + 2:3, 99 + 4:5, 3)
z
```

[.feemcube *Extract or replace parts of FEEM cubes*

Description

Extract or replace single intensities, vectors of them, whole FEEM spectra or even data cubes or their parts from a FEEM cube.

Usage

```
  ## S3 method for class 'feemcube'
x[i, j, k, drop = TRUE]
  ## S3 replacement method for class 'feemcube'
x[i, j, k] <- value
```

Arguments

x	A FEEM cube object.
i, j, k	Row, column and sample indices, respectively. As usual, may be integer, logical or character vectors. Omitting a parameter results in choosing the whole axis.
drop	Coerce result to the lowest possible dimension (dropping the feemcube class).

value   An array-like object to assign values from. When assigning from FEEM or
                         FEEM cube objects, wavelengths are required to match and warnings are issued
                         if scale factors don't match. Use vector subsetting (zero or one argument inside
                         the brackets) to disable the check.

Value

For [: If choosing multiple values along each axis or `drop` is `FALSE`, a FEEM cube object. If
choosing only one sample but multiple wavelengths, a FEEM object. Otherwise, a named numeric
matrix or vector, depending on the dimensions chosen.

For [<-: a FEEM cube object.

See Also

feemcube, [.feem

Examples

```
z <- feemcube(array(1:385, c(5, 7, 11)), 1:5, 1:7, 1:11)
str(z[1:4, 1:2, 1:2])
z[2:3, 4:5, 3] <- feem(matrix(1:4, 2), 2:3, 4:5, 3)
z[,,3]
```

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