Package 'USGSHydroOpt'

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Type Package

Title Tools for optical data analysis

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Description Tools for optical data analysis

License file LICENSE

Depends R (>= 3.0)

Imports reshape2

LazyLoad yes

LazyData yes

VignetteBuilder knitr

R topics documented:

`a` *a*

Description

Example data a. An array with 3-D fluoresence results. The 3 dimensions are the excitation wavelength (character), the emission wavelength (character), and the sample number, e.g.,"GRnumber" (character).

Author(s)

Steve Corsi <srcorsi@usgs.gov>

`dfabs` *dfabs*

Description

Example data dfabs. This dataframe contains the absorbance spectra for 265 samples. The wavelength is measured from 200nm to 750nm for each sample. One column called "wavelengths" contains the wavelength for the absorbance measurment in nm.

Author(s)

Steve Corsi <srcorsi@usgs.gov>

`dfFluor` *dfFluor*

Description

Example data dfFluor. Contains vectorized fluoresence data and one column called "Wavelength.Pairs" which contains the Excitation and Emission wavelengths defined in this format: ###/###. For example, Excitation 250 and emmission 400 would be represented as "250/400".

Author(s)

Steve Corsi <srcorsi@usgs.gov>

dfsags *dfsags*

Description

Example data dfsags. This dataframe contains three columns. The first two columns contain the lower and upper wavelength in nm (as integer) for which a spectral slope is to be calculated for each sample. The third column "Name" contains the name of the spectral slope which can then be used as a summary optical variable.

Author(s)

Steve Corsi <srcorsi@usgs.gov>

dfsummary *dfsummary*

Description

Example data dfsummary. Contains summary optical variables for each sample, here called "GR-number". These summary optical variables are computed using the functions in this package.

Author(s)

Steve Corsi <srcorsi@usgs.gov>

ex_ems *ex_ems*

Description

Example data ex_ems. This dataframe contains three columns. The first column called "Peak" contains the character name of the EEMs peak. The second column called "ExCA" contains the excitation wavelength for a particular peak as type integer. The third column called "EmCA" contains the emission wavelength for a particular peak as type integer.

Author(s)

Steve Corsi <srcorsi@usgs.gov>

getAbs *getAbs*

Description

Retrieves individual absorbance coefficients

Usage

```
getAbs(dataAbs, waveCol, wavs, colSubsetString, dataSummary, grnum)
```

Arguments

dataAbs	dataframe with absorbance spectra results, one column per sample, and one column with the wavelengths.
waveCol	character column name to define the wavelengths for which absorbance was measured.
wavs	numeric vector with absorbance wavelengths to extract.
colSubsetString	unique characters to identify which columns have absorbance data. The default is "gr" to comply with the common naming from the CA WSC.
dataSummary	dataframe with summary absorbance and fluoresence data. This function adds columns to the end of this dataframe as additional summary data.
grnum	character column name that defines the grnumbers in the dataSummary dataframe. These names are used to merge spectral slope data into the summary dataframe. This function assumes the column names of the dataAbs are grnumbers as well.

Value

summary absorbance and fluoresence dataframe with the additional absorbance peaks extracted using getAbs

Examples

```
dataAbs <- dfabs
waveCol <- "wavelengths"
wavs <- c(430,530,630,730)
colSubsetString <- "gr"
dataSummary <- dfsummary
grnum <- "GRnumber"
testAbs <- getAbs(dataAbs,waveCol,wavs,
               colSubsetString,dataSummary,grnum)
```

getExpResid *getSag*

Description

Computes spectral slopes from absorbance data using a linear regression to determine the first order decay function as defined in Helms et al. 2008, Limnol. Oceanogr., 53(3), 955-969. aL = aRef * exp(-S*(L-LRef)) where a = absorbance coefficient, S = spectral slope, and L = wavelength. Function assumes that the column names of the absorbance data file being used are formatted as grnumbers.

Usage

```
getExpResid(wavelength, rangeReg, rangeGap, dataAbs, waveCol, colSubsetString,
  dataSummary, grnum)
```

Arguments

wavelength	absorbance numeric wavelength
rangeReg	numeric string with absorbance wavelength range to be considered for computing spectral slope
rangeGap	numeric string with the absorbance wavelength range for which decay function should be applied
dataAbs	dataframe with absorbance spectra results, one column per sample
waveCol	character column name to define the wavelengths for which absorbance was measured
colSubsetString	character with unique letters to identify which columns have absorbance data. The default is "gr" to comply with the common naming from the CA WSC
dataSummary	dataframe with summary absorbance and fluoresence data. This function adds columns to the end of this dataframe as additional summary data.
grnum	character column name that defines the grnumbers in the dataSummary dataframe.

Value

dataframe with the added spectral slope for each sample and plots with the absorbance spectra for rangeReg showing the model constructed using the spectral slope (red); and the absorbance data where black = the data in rangeReg that is not in rangeGap and blue = the data from rangeGap.

Examples

```
wavelength <- 267
rangeReg <- c(240,340)
rangeGap <- c(255,300)
dataAbs <- dfabs
waveCol <- "wavelengths"
colSubsetString <- "gr"
dataSummary <- dfsummary
grnum <- "GRnumber"
testdfOpt <- getExpResid(wavelength,rangeReg,rangeGap,dataAbs,waveCol,
                    colSubsetString,dataSummary,grnum)
```

getIndexes *getIndexes*

Description

Computes humification index and fluorescence indes from fluorescence data. HIX as defined by Ohno, 2002, Fluorescence inner-filtering correction for determining the humification index of dissolved organic matter. Environ. Sci. Technol. 36: 742-746 doi: 10.1021/es0155276, HIX = sum(I435:I480)/(sum(I300:I345)+sum(I435:I480)) for ex=254 and FI_2005 as defined by Cory and McKnight, 2005, Fluorescence spectroscopy reveals ubiquitous presence of oxidized and reduced quinones in DOM. Environ. Sci. Technol. 39: 8142-8149, doi:10.1021/es0506962 and FI_2001 defined by MCKNIGHT, D. M., E. W. BOYER, P. K. WESTERHOFF, P. T. DORAN, T. KULBE, AND D. T. ANDERSEN. 2001. Spectrofluorometric characterization of DOM for indication of precursor material and aromaticity. Limnol. Oceanogr. 46: 38-48, doi:10.4319/lo.2001.46.1.0038. FI = ex370em470/ex370em520 and freshness index as defined by PARLANTI, E., K. WORZ, L. GEOFFROY, AND M. LAMOTTE. 2000. Dissolved organic matter fluorescence spectroscopy as a tool to estimate biological activity in a coastal zone submitted to anthropogenic inputs. Org. Geochem. 31: 1765-1781, doi:10.1016/S0146-6380(00)00124-8 FreshI = ex310em380/max(ex310 between em470 and em520),

Usage

```
getIndexes(a, dataSummary, grnum)
```

Arguments

a	an array with 3-D fluorescence results. The 3 dimensions are the excitation wavelength (character), the emission wavelength (character), and the sample number (character).
dataSummary	dataframe with summary absorbance and fluoresence data. This function adds columns to the end of this dataframe as additional summary data.
grnum	character column name that defines the grnumbers (sample numbers) in the dataSummary dataframe. These names are used to merge spectral slope data into the summary dataframe. This function assumes the column names of the dataAbs are grnumbers as well.

Value

dataSummary dataframe with the additional columns containing the humification and fluoresence indices.

Examples

```
a <- a
dataSummary <- dfsummary
dataSummary <- dataSummary[,-c(43:46)] #remove columns with fluoresence and humic index
grnum <- "GRnumber"
test1 <- getIndexes(a,dataSummary,grnum)
```

getLog10 *getLog10*

Description

Computes log transform of optical summary data.

Usage

```
getLog10(dataSummary, signals, grnum)
```

Arguments

dataSummary	dataframe with summary absorbance and fluoresence data.
signals	character vector of variable names in dataSummary for generating log transforms
grnum	character column name that defines the grnumbers in the dataSummary dataframe. These names are used to merge ratio data into the summary dataframe.

Value

dataframe with the log 10 transform of the summary absorbance and fluoresence data.

Examples

```
dataSummary <- dfsummary
signals <- ratioSignals[which(ratioSignals[2]>0),1]
grnum<-"GRnumber"
test2 <- getLog10(dataSummary,signals,grnum)
```

getMeanFl *getMeanFl*

Description

and freshness index as defined by PARLANTI, E., K. WORZ, L. GEOFFROY, AND M. LAMOTTE. 2000. Dissolved organic matter fluorescence spectroscopy as a tool to estimate biological activity in a coastal zone submitted to anthropogenic inputs. Org. Geochem. 31: 1765-1781, doi:10.1016/S0146-6380(00)00124-8 FreshI = ex310em380/max(ex310 between em470 and em520)

Usage

```
getMeanFl(a, signals, Peak, Ex1, Ex2, Em1, Em2, dataSummary, grnum)
```

Arguments

a	an array with 3-D fluorescence results. The 3 dimensions are the excitation wavelength (character), the emission wavelength (character), and the sample number (character). This function assumes names of the third dimension in this array are sample numbers (GRnumber)
signals	dataframe defining the max and min excitation (integer) and the max and min emmission (integer) wavelengths for which to compute averages. Contains one column (character) with the names of the various parameters (e.g.,OB1,S1.50,B,T).
Peak	character column for the column in signals with parameters to be computed
Ex1	the first integer excitation wavelength in the range
Ex2	the second integer excitation wavelength in the range. This can be blank if one specific excitation wavelength is used.
Em1	the first integer emmission wavelength in the range
Em2	the second integer emmission wavelength in the range. This can be blank if one specific emmission wavelength is used.
dataSummary	dataframe with summary absorbance and fluoresence data. This function adds columns to the end of this dataframe as additional summary data.
grnum	character column name that defines the grnumbers in the dataSummary dataframe.

Value

dataSummary dataframe with the additional freshness index columns.

Examples

```
a <- a
signals <- signals
Peak <- "Peak"
Ex1 <- "Ex1"
Ex2 <- "Ex2"
Em1 <- "Em1"
Em2 <- "Em2"
dataSummary <- dfsummary
grnum <- "GRnumber"
testMeanFl <- getMeanFl(a,signals,Peak,Ex1,Ex2,Em1,Em2,dataSummary,grnum)
```

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getRatios *getRatios*

Description

Computes ratios from optical data. Assumes that the signal with the greatest mean is in the numerator making the mean ratio greater than one.

Usage

```
getRatios(dataSummary, sigs, grnum)
```

Arguments

dataSummary	dataframe with summary absorbance and fluoresence data. This
sigs	signals vector of variable names in dataSummary for generating ratios
grnum	Column name that defines the grnumbers in the dataSummary dataframe. These names are used to merge ratio data into the summary dataframe.

Value

dataSummary dataframe with the additional columns of spectral ratios computed using getRatios

Examples

```
dataSummary <- dfsummary
sigs <- ratioSignals[which(ratioSignals[2]>0),1]
grnum <- "GRnumber"
test <- getRatios(dataSummary,sigs,grnum)
```

---

getSag *getSag*

Description

Computes spectral slopes from absorbance data using a linear regression to determine the first order decay function as defined in Helms et al. 2008, Limnol. Oceanogr., 53(3), 955-969. aL = aRef * exp(-S*(L-LRef)) where a = absorbance coefficient, S = specral slope, and L = wavelength.

Usage

```
getSag(dataAbs, waveCol, sag, colSubsetString, dataSummary, grnum)
```

Arguments

dataAbs	dataframe with absorbance spectra results, one column per sample (e.g.,GRnumber)
waveCol	column name as character to define the wavelengths (as integer) for which absorbance was measured
sag	dataframe with three columns. The first column represents the low wavelength (as integer), the second column represents the high wavelength (as integer) for which spectral slopes are to be defined, and the third column is the variable name to be used (as factor). A spectral slope is computed for each row.
colSubsetString	unique characters to identify which columns have absorbance data. The default is "gr" to comply with the common naming from the CA WSC
dataSummary	dataframe with summary absorbance and fluoresence data. This function adds columns to the end of this dataframe as additional summary data.
grnum	column name as character that defines the grnumbers in the dataSummary dataframe. These names are used to merge spectral slope data into the summary dataframe. This function assumes the column names of the dataAbs are grnumbers as well.

Value

dataSummary dataframe with the additional columns containing spectral slopes as defined in sag for each sample (e.g., GRnumber).

Examples

```
dataAbs <- dfabs
waveCol <- "wavelengths"
sag <- dfsags
colSubsetString <- "gr"
dataSummary <- dfsummary
dataSummary <- dataSummary[,-c(64:67)] #remove columns with spectral slopes and re-compute with this function
grnum <- "GRnumber"
testSag <- getSag(dataAbs,waveCol,sag,colSubsetString,dataSummary,grnum)
```

`plotEEMs2` *plotEEMs2*

Description

Plot contour graph of excitation emmission spectra with defined peaks indicated on the graph

Usage

```
plotEEMs2(mat, Ex, Em, nlevels, Peaks, peakCol, peakEx, peakEm, mainTitle)
```

Arguments

`mat`	2-D matrix of excitation-emmission spectra
`Ex`	numeric excitation wavelengths
`Em`	numeric emmission wavelengths
`nlevels`	numeric color levels for contour graph. 50 is commonly used for a value here.
`Peaks`	dataframe with peaks to be indicated on the graph
`peakCol`	character column name in Peaks which contains the abbreviation for that peak
`peakEx`	character column name in Peaks to use for excitation wavelengths
`peakEm`	character column name in Peaks to use for emmission wavelengths
`mainTitle`	Plot title

Value

Excitation-Emission (EEMs) Plot with the important peaks identified

Examples

```
GRnum <- "gr15222"
mat <- a[,,GRnum]
Ex <- as.numeric(names(a[,1,1]))
Em <- as.numeric(names(a[1,,1]))
nlevels <- 50
Peaks <- ex_ems
peakCol <- "Peak"
peakEx <- "ExCA"
peakEm <- "EmCA"
mainTitle <- "Example EEMs Plot"
exampleEEMs <- plotEEMs2(mat=mat,Ex=Ex,Em=Em,nlevels=nlevels,Peaks=Peaks,peakCol=peakCol,
peakEx=peakEx,peakEm=peakEm,mainTitle=mainTitle)
```

`ratioSignals` *ratioSignals*

Description

Example data ratioSignals. Contains one column "ratioSignals" with the name of the different optical metrics used as signals for different chemical species in freshwater.

Author(s)

Steve Corsi <srcorsi@usgs.gov>

`signals` *signals*

Description

Example data signals. Contains one column called "Peak" with different excitation-emission peaks that act as signals for particular chemical species. These peaks are well characterized and the "Source" column in this dataframe lists the source that characterized each excitation-emission peak and the chemical species that it identifies. There are four additional columns with the Excitation and Emission wavelengths for each peak.

Author(s)

Steve Corsi <srcorsi@usgs.gov>

VectorizedTo3DArray *VectorizedTo3DArray*

Description

Converts vectorized fluorescence dataframe into a 3-D array with Ex, Em, and GRnumber as the dimensions. This results in one 2-D excitation-emmission array per sample. Requires the reshape2 package.

Usage

```
VectorizedTo3DArray(df, ExEm)
```

Arguments

df	dataframe with vectorized fluorescence data in the format from the CA WSC with one column containing both the Excitation and Emission pair, and all other columns representing a sample (e.g.,GRnumber)
ExEm	the character name of column with Excitation and Emmission wavelengths defined in this format: ###/###. For example, Excitation 250 and emmission 400 would be represented as "250/400".

Value

an array with 3-D fluorescence results. The 3 dimensions are the excitation wavelength (character), the emission wavelength (character), and the sample number, e.g.,"GRnumber" (character).

Examples

```
df <- dfFluor
ExEm <- "Wavelength.Pairs"
aTest <- VectorizedTo3DArray(df,ExEm)
```

Index