

Package ‘spectratrait’

February 3, 2021

Title A simple add-on package to aid in the fitting of leaf-level spectra-trait PLSR models

Version 0.9.9

Maintainer Shawn P. Serbin <sserbin@bnl.gov>

Description Provides functions to conduct standardized leaf-level spectra-trait PLSR model fitting including uncertainty analysis that follow DOI: <https://doi.org/10.1111/nph.16123>

License MIT + file LICENSE

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.1

Imports httr (>= 1.4.2),
readr (>= 1.3.1),
pls (>= 2.7-2),
dplyr (>= 1.0.1),
reshape2 (>= 1.4.4),
here (>= 0.1),
plotrix (>= 3.7-8),
ggplot2 (>= 3.3.2),
gridExtra (>= 2.3)

Suggests devtools (>= 2.3.1),
remotes (>= 2.2.0),
RCurl (>= 1.98-1.2),
scales (>= 1.1.1)

Depends R (>= 2.10)

VignetteBuilder knitr

NeedsCompilation no

R topics documented:

create_data_split	2
f.coef.valid	3
f.plot.coef	3
f.plot.spec	4
find_optimal_components	5
get_ecosis_data	6

pls_permutation	6
source_GitHubData	7
testForPackage	7
VIP	8
VIPjh	8
Index	9

create_data_split	<i>Create a calibration (training) / validation data split for PLSR model fitting and testing</i>
-------------------	---

Description

Create a calibration (training) / validation data split for PLSR model fitting and testing

Usage

```
create_data_split(
  dataset = NULL,
  approach = NULL,
  split_seed = 123456789,
  prop = 0.8,
  group_variables = NULL
)
```

Arguments

dataset	input full PLSR dataset to split into cal/val datasets
approach	approach to splitting the dataset. Options: base or dplyr
split_seed	random seed to use for splitting data
prop	the proportion of data to preserve for calibration (e.g. 0.8) and validation (0.2). This sets the calibration proportion
group_variables	Use factor variables to conduct a stratified sampling for cal/val

Value

output_list A list containing the calibration dataset (cal_data) and validation dataset (val_data)

Author(s)

Julien Lamour, Jeremiah Anderson, Shawn P. Serbin

f.coef.valid	<i>f.coef.valid</i>
--------------	---------------------

Description

f.coef.valid

Usage

```
f.coef.valid(plsr.out, data_plsr, ncomp, inVar)
```

Arguments

plsr.out	plsr model obtained with jaccknife = TRUE
data_plsr	data used for the plsr model with Spectra the matrix of spectra
ncomp	number of selection components
inVar	Name of the PLSR model response variable

Value

B returns the intercept and the coefficients of the jackknife or bootstrap validation

Author(s)

Julien Lamour

f.plot.coef	<i>f.plot.coef</i>
-------------	--------------------

Description

f.plot.coef

Usage

```
f.plot.coef(  
  Z,  
  wv,  
  xlim = NULL,  
  position = "topright",  
  type = "Coefficient",  
  plot_label = NULL  
)
```

Arguments

<code>Z</code>	Coefficient matrix with each row corresponding to the coefficients and wavelength in columns
<code>wv</code>	vector of wavelengths
<code>xlim</code>	vector to change the default xlim of the plots (ex <code>xlim = c(500, 2400)</code>)
<code>position</code>	Position of the legend (see base function legend for help)
<code>type</code>	Name of the y axis and of the legend
<code>plot_label</code>	optional plot label to include with the figure

Author(s)

Julien Lamour

<code>f.plot.spec</code>	<i>f.plot.spec</i>
--------------------------	--------------------

Description

`f.plot.spec`

Usage

```
f.plot.spec(
  Z,
  wv,
  xlim = NULL,
  position = "topright",
  type = "Reflectance",
  plot_label = NULL
)
```

Arguments

<code>Z</code>	Spectra matrix with each row corresponding to a spectra and wavelength in columns
<code>wv</code>	vector of wavelengths corresponding to the column of the spectra matrix <code>Z</code>
<code>xlim</code>	vector to change the default xlim of the plots (ex <code>xlim = c(500, 2400)</code>)
<code>position</code>	Position of the legend (see base function legend for help)
<code>type</code>	Name of the y axis and of the legend. E.g. Reflectance, Transmittance
<code>plot_label</code>	optional plot label to include with the figure

Author(s)

Julien Lamour, Shawn P. Serbin

`find_optimal_components`*Apply different methods to determining the optimal number of PLSR model components*

Description

Apply different methods to determining the optimal number of PLSR model components

Usage

```
find_optimal_components(  
  dataset = NULL,  
  method = "pls",  
  maxComps = 20,  
  iterations = 20,  
  seg = 100,  
  prop = 0.7,  
  random_seed = 123456789  
)
```

Arguments

<code>dataset</code>	input full PLSR dataset. Usually just the calibration dataset
<code>method</code>	Which approach to use to find optimal components. Options: <code>pls</code> , <code>firstPlateau</code> , <code>firstMin</code>
<code>maxComps</code>	maximum number of components to consider
<code>iterations</code>	how many different permutations to run
<code>seg</code>	For the built-in <code>pls</code> method, how many different data segments to select from the input dataset
<code>prop</code>	proportion of data to preserve for each permutation
<code>random_seed</code>	random seed to use for splitting data

Value

`nComps` the optimal number of PLSR components

Author(s)

Julien Lamour, Jeremiah Anderson, Shawn P. Serbin

get_ecosis_data	<i>Function to pull data from EcoSIS using the EcoSIS API</i>
-----------------	---

Description

Function to pull data from EcoSIS using the EcoSIS API

Usage

```
get_ecosis_data(ecosis_id = NULL)
```

Arguments

ecosis_id the alphanumeric EcoSIS API dataset ID

Value

EcoSIS spectral dataset object

Author(s)

Shawn P. Serbin, Alexey Shiklomanov

Examples

```
## Not run:
ecosis_id <- "960dbb0c-144e-4563-8117-9e23d14f4aa9"
dat_raw <- get_ecosis_data(ecosis_id = ecosis_id)
head(dat_raw)
names(dat_raw)[1:40]

## End(Not run)
```

pls_permutation	<i>Run a PLSR model permutation analysis. Can be used to determine the optimal number of components or conduct a bootstrap uncertainty analysis</i>
-----------------	---

Description

See Serbin et al. (2019). DOI: <https://doi.org/10.1111/nph.16123>

Usage

```
pls_permutation(
  dataset = NULL,
  maxComps = 20,
  iterations = 20,
  seg = 100,
  prop = 0.7
)
```

Arguments

dataset	input full PLSR dataset. Usually just the calibration dataset
maxComps	maximum number of components to use for each PLSR fit
iterations	how many different permutations to run
seg	currently unused - should be removed from this function call
prop	proportion of data to preserve for each permutation

Author(s)

Julien Lamour, Shawn P. Serbin

source_GitHubData	<i>Function to source text data from GitHub</i>
-------------------	---

Description

Function to source text data from GitHub

Usage

```
source_GitHubData(url, sep = ",", header = TRUE)
```

Arguments

url	http/https URL to the github dataset
sep	dataset file delimiter
header	TRUE/FALSE does the file have a column header?

Author(s)

gist.github.com/christophergandrud/4466237

testForPackage	<i>Function to check for installed package not presently used</i>
----------------	---

Description

Function to check for installed package not presently used

Usage

```
testForPackage(pkg)
```

VIP	<i>VIP returns all VIP values for all variables and all number of components, as a ncomp x nvars matrix.</i>
-----	--

Description

VIP returns all VIP values for all variables and all number of components, as a ncomp x nvars matrix.

Usage

VIP(object)

VIPjh	<i>VIPjh returns the VIP of variable j with h components</i>
-------	--

Description

VIPjh returns the VIP of variable j with h components

Usage

VIPjh(object, j, h)

Index

`create_data_split`, [2](#)

`f.coef.valid`, [3](#)

`f.plot.coef`, [3](#)

`f.plot.spec`, [4](#)

`find_optimal_components`, [5](#)

`get_ecosis_data`, [6](#)

`pls_permutation`, [6](#)

`source_GitHubData`, [7](#)

`testForPackage`, [7](#)

VIP, [8](#)

VIPjh, [8](#)