Package 'FieldSpec'

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Type Package

Title Functions for processing field spectroscopy data

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Description A field spectroscopy package containing functions to process spectral files collected with an Analytical Spectral Devices (ASD) or Spectral Evolution instrument. The goal is to streamline and standardize spectral data processing for use in remote sensing, ecology, and plant ecophysiological research.

Depends XML, Hmisc

Suggests testthat, Rprospect, signal

SystemRequirements

OS_type Windows, unix, mac

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LazyLoad yes

LazyData FALSE

Collate 'import.asd.R' 'read.asd.R' 'spec.utils.R' 'average.spec.R''jump.correction.R' 'average.spec.se.R'

R topics documented:

`average.spec` *average replicate spectra within a directory of spectra files*

Description

Function to average replicate spectra within a directory of spectra files

Usage

```
average.spec(file.dir = NULL, out.dir = NULL,
  start.wave = NULL, end.wave = NULL, step.size = NULL,
  bias.threshold = NULL, suffix.length = NULL,
  output.file.ext = NULL, metadata.file = NULL,
  image = FALSE, settings.file = NULL)
```

Arguments

`file.dir`	Directory of spectra files to process
`out.dir`	Output directory for processed spectra files
`start.wave`	Starting wavelength of spectra files. Not needed if specified in XML settings file.
`end.wave`	Ending wavelength of spectra files. Not needed if specified in XML settings file.
`step.size`	Resolution of spectra files. E.g. 1 for 1nm, 5 for 5nm. Not needed if specified in XML settings file.
`bias.threshold`	Reflectance/transmittance cutoff to remove spectra with anartificial bias (shift) due to improper spectral collection
`suffix.length`	Length of auto numbering attached to ASD file names. This number of characters will be removed from the filename when averaged.
`output.file.ext`	Optional setting to set file extension of output files. Defaults to .csv
`spec.dataframe`	Option to return a data frame with the converted spectra files
`metadata.file`	Option to select custom metadata file for use in processing. If not set then the information is either read from default metadata file, the settings file or at the function call. Need to set this as the full qualified path to the spectral metadata file is using a custom file/location
`image`	Logical. Whether to produce .png images of each spectrum (TRUE) or not (FALSE). Default is FALSE. Useful for diagnosing spectral observations during processing.
`settings.file`	Settings file used for spectral processing options (OPTIONAL). Contains information related to the spectra collection instrument, output directories, and processing options such as applying a jump correction to the spectra files. Options in the settings file take precedent over options selected in the function call.

Author(s)

Shawn P. Serbin

Examples

```
## Not run:
average.spec()
average.spec(file.dir,out.dir, start.wave=350,end.wave=2500,step.size=1,bias.threshold=0.06,
suffix.length=5,output.file.ext=".csv",spec.dataframe = TRUE,)

## End(Not run)
```

`average.spec.se` *average replicate spectra within a directory of spectra files*

Description

Function to average replicate spectra within a directory of spectra files

Usage

```
average.spec.se(file.dir = NULL, out.dir = NULL,
  spec.type = NULL, spec.file.ext = NULL,
  start.wave = NULL, end.wave = NULL, step.size = NULL,
  bias.threshold = NULL, suffix.length = NULL,
  output.file.ext = NULL, settings.file = NULL)
```

Arguments

`file.dir`	directory of spectra files to process
`out.dir`	output directory for processed spectra files
`spec.type`	Option to set what type of spectra to average. Options: Reflectance, Transmittance. Can be set with abbreviations: e.g. "Refl" or "Tran" Default is "Reflectance"
`spec.file.ext`	Optional to set the input file extension. Default is ".sed"
`start.wave`	starting wavelength of spectra files. Not needed if specified in XML settings file.
`end.wave`	ending wavelength of spectra files. Not needed if specified in XML settings file.
`step.size`	resolution of spectra files. E.g. 1 for 1nm, 5 for 5nm. Not needed if specified in XML settings file.
`bias.threshold`	reflectance/transmittance cutoff to remove spectra with anartificial bias (shift) due to improper spectral collection
`suffix.length`	length of auto numbering attached to ASD file names. This number of characters will be removed from the filename when averaged.
`output.file.ext`	optional setting to set file extension of output files. Defaults to .csv
`settings.file`	settings file used for spectral processing options (OPTIONAL). Contains information related to the spectra collection instrument, output directories, and processing options such as applying a jump correction to the spectra files. Options in the settings file take precedent over options selected in the function call.

Author(s)

Shawn P. Serbin

`concat.spectra` *Concatenate a directory of spectra files into a single .csv file. Works on a single directory or a series of directories*

Description

Concatenate a directory of spectra files into a single .csv file. Works on a single directory or a series of directories

Usage

```
concat.spectra(file.dir = NULL, out.dir = NULL,
  out.filename = NULL, in.file.ext = ".csv",
  out.file.ext = ".csv", transpose = FALSE,
  spec.dataframe = FALSE)
```

Arguments

`file.dir`	directory of spectra files to process. Currently works on spectra files formatted where each row is a wavelength and associated spectral observation.
`out.dir`	output directory for concatenated spectra files. If not set then the output directory defaults to file.dir (input directory)
`out.filename`	filename for concatenated spectra files
`in.file.ext`	file extension for individual spectra files. Defaults to ".csv"
`out.file.ext`	option to set the output extension. Defaults to ".csv"
`transpose`	option to transpose the spectra to/from row/column major output. This will be applied to both the returned dataframe (optional) and output file. TRUE/FALSE. Default FALSE
`spec.dataframe`	option toreturn a R dataframe containing the concatenated spectral data. TRUE/FALSE

Author(s)

Shawn P. Serbin

Examples

```
## Not run:
concat.spectra()
spectra <- concat.spectra(file.dir=file.dir,out.dir=out.dir,out.filename="concat.spectra",
out.file.ext=".csv",transpose=FALSE,spec.dataframe=FALSE)

## End(Not run)
```

`extract.metadata` *Extract metadata for each spectra sample. Works on a single spectra or a directory.*

Description

Extract metadata for each spectra sample. Works on a single spectra or a directory.

Usage

```
extract.metadata(file.dir = NULL, out.dir = NULL,
  instrument = NULL, spec.file.ext = NULL,
  output.file.ext = ".csv", tz = NULL,
  settings.file = NULL)
```

Arguments

`file.dir`	File directory or filename of single spectra for processing
`out.dir`	Output directory for metadata information file
`instrument`	What instrument was used to collect spectra. Current options: ASD, SE
`spec.file.ext`	[Optional] Input spectra file extension. E.g. .asd (ASD) or .sed (Spectral Evolution). Default for ASD instruments is .asd. Default for Spectral Evolution instruments is .sed
`output.file.ext`	[Optional] Output file extension of metadata information file. Default .csv
`tz`	[Optional] Set the timezone of the spectra file collection. Used to covert spectra collection time to UTC. If unused it is assumed that the correct timezone is the current system timezone.
`settings.file`	[Optional] Spectral settings file

Value

output Returns a dataframe of spectral metadata information

Author(s)

Shawn P. Serbin

Examples

```
# ASD
file <- system.file("extdata/PM01_TIAM_B_LC_REFL00005.asd",package="FieldSpec")
output <- extract.metadata(file,instrument="ASD")

# Spectral Evolution
file <- system.file("extdata/cvars_grape_leaf1_lc_rg_01236.sed",package="FieldSpec")
output <- extract.metadata(file,instrument="SE")
```

`extract.metadata.asd` *Extract metadata from raw binary ASD files. Called from extract.metadata*

Description

Extract metadata from raw binary ASD files. Called from extract.metadata

Usage

```
extract.metadata.asd(file.dir, out.dir, spec.file.ext,
  output.file.ext, tz)
```

Arguments

`file.dir`	File directory or filename of single spectra for processing
`out.dir`	Output directory for meta-data information file
`spec.file.ext`	[Optional] Input spectra file extension. E.g. .asd (ASD) or .sed (Spectral Evolution). Default for ASD instruments is .asd. Default for Spectral Evolution instruments is .sed
`output.file.ext`	[Optional] Output file extension of meta-data information file. Default .csv
`tz`	[Optional] Set the timezone of the spectra file collection. Used to covert spectra collection time to UTC. If unused it is assumed that the correct timezone is the current system timezone.

Value

output Returns output dataframe of ASD metadata information

Author(s)

Shawn P. Serbin

`extract.metadata.se` *Extract metadata from Spectral Evolution files. Called from extract.metadata*

Description

Extract metadata from Spectral Evolution files. Called from extract.metadata

Usage

```
extract.metadata.se(file.dir, out.dir, spec.file.ext,
  output.file.ext, tz)
```

Value

output Returns output dataframe of SE metadata information

Author(s)

Shawn P. Serbin

`import.asd` *Import raw binary ASD spectra files*

Description

A wrapper function to import raw binary ASD spectra files, apply jump correction to the imported files and average replicate files into a single spectrum. Calls read.asd(), jump.correction(), and average.spec() functions.

Usage

```
import.asd(asd.dir = NULL, output.dir = NULL,
  jump.correction = FALSE, average = FALSE,
  start.wave = NULL, end.wave = NULL, step.size = NULL,
  jumploc1 = NULL, jumploc2 = NULL, asd.file.ext = NULL,
  output.file.ext = NULL, settings.file = NULL)
```

Arguments

`asd.dir`	directory containing raw ASD files or sub-directories to be processed. Not needed if specified in settings file.
`output.dir`	main ouput directory. Not needed if specified in settings file.
`jump.correction`	option to apply a jump correction to the imported spectra files. Not needed if specified in settings file.
`average`	option to average imported spectra files. Will use jump corrected files if exist. Not needed if specified in settings file.
`start.wave`	starting wavelength of spectra files. Not needed if specified in settings file.
`end.wave`	ending wavelength of spectra files. Not needed if specified in settings file.
`step.size`	resolution of spectra files. E.g. 1 for 1nm, 5 for 5nm. Not needed if specified in settings file.
`jumploc1`	location of the first jump in the spectra to correct. Not needed if jump.correction=FALSE or if specified in settings file.
`jumploc2`	location of the second jump in the spectra to correct. Not needed if jump.correction=FALSE or if specified in settings file.
`asd.file.ext`	file extension for input binary asd spectra files
`output.file.ext`	optional setting to set file extension to output files. Defaults to .csv
`settings.file`	settings file used for spectral processing options (OPTIONAL). Contains information related to the spectra collection instrument, output directories, and processing options such as applying a jump correction to the spectra files. Options in the settings file take precedent over options selected in the function call.

Author(s)

Shawn P. Serbin

`jump.correction` *apply a jump (splice) correction to imported ASD spectra files. This splice or jump occurs at the boundaries between detectors*

Description

A function to apply a jump (splice) correction to imported spectra files

Usage

```
jump.correction(file.dir = NULL, out.dir = NULL,
  spec.type = NULL, start.wave = NULL, end.wave = NULL,
  step.size = NULL, jumploc1 = NULL, jumploc2 = NULL,
  firstJumpMax = NULL, secondJumpMax = NULL,
  output.file.ext = NULL, metadata.file = NULL,
  image = FALSE, settings.file = NULL)
```

Arguments

`file.dir`	directory of spectra files to process
`out.dir`	output directory for processed spectra files
`spec.type`	[Optional] Option to set the type of spectra being processed. Options: "Reflectance" or "Transmittance" Defaults to "Reflectance"
`start.wave`	starting wavelength of spectra files. Not needed if specified in XML settings file.
`end.wave`	ending wavelength of spectra files. Not needed if specified in XML settings file.
`step.size`	resolution of spectra files. E.g. 1 for 1nm, 5 for 5nm. Not needed if specified in settings file.
`jumploc1`	Wavelength location of the first jump in the spectra to correct. Not needed if specified in XML settings file.
`jumploc2`	Wavelength location of the second jump in the spectra to correct. Not needed if specified in XML settings file.
`firstJumpMax`	maximum jump threshold for the first jump location. Determines whether spectra will be corrected or flaged as bad. (Optional. Default is 0.02)
`secondJumpMax`	maximum jump threshold for the second jump location. Determines whether spectra will be corrected or flaged as bad. (Optional. Default is 0.02)
`output.file.ext`	option to set file extension of the output files. Defaults to .csv
`metadata.file`	Option to select custom metadata file for use in processing. If not set then the information is either read from default metadata file, the settings file or at the function call. Need to set this as the full qualified path to the spectral metadata file is using a custom file/location
`image`	Logical. Whether to produce .png images of each spectrum (TRUE) or not (FALSE). Default is FALSE. Useful for diagnosing spectral observations during processing.
`settings.file`	settings file used for spectral processing options (OPTIONAL). Contains information related to the spectra collection instrument, output directories, and processing options such as applying a jump correction to the spectra files.

Value

output list containing processed spectra and associated diagnostic information

Author(s)

Shawn P. Serbin

Examples

```
## Not run:
jump.correction(file.dir,out.dir='~', start.wave=350,end.wave=2500,step.size=1,jumploc1=651,jumploc2=1451,
output.file.ext=".csv",settings.file=NULL)

## End(Not run)
```

---

read.asd *A function to import raw ASD binary files*

Description

A function to import raw ASD binary files to ascii flat file format

Usage

```
read.asd(file.dir = NULL, out.dir = NULL,
  spec.type = NULL, start.wave = NULL, end.wave = NULL,
  step.size = NULL, image = FALSE,
  spec.file.ext = ".asd", output.file.ext = ".csv",
  get.metadata = TRUE, settings.file = NULL)
```

Arguments

file.dir	A single ASD binary file or directory of ASD files to import. Currently only supports single directory processing (i.e. no nested dir structures)
out.dir	Main output directory for processed spectra files. If not set then no output ASCII files are provided. If set then output ASCII files for each spectra are written to out.dir/ascii_files
spec.type	Optional. Option to set the type of spectra being processed. Options: "Reflectance" or "Transmittance" Defaults to "Reflectance"
start.wave	Optional. Selected starting wavelength of ASD binary spectra files. Depends on instrument. If not set then read from file header
end.wave	Optional. Selected ending wavelength of ASD binary spectra files. Depends on instrument. If not set then read from file header
step.size	Optional. Wavelength step size for ASD files. E.g. 1nm, 5nm, 10nm If not set then read from file header. If selected for larger size than raw data, spectrum is interpolated (not yet availible)
image	Logical. Whether to produce .png images of each spectrum (TRUE) or not (FALSE). Default is FALSE. Useful for diagnosing spectral observations during processing.

spec.file.ext	file extension of ASD files. Usually ".asd" (Default)
output.file.ext	optional setting to set file extension to output files. Defaults to .csv
get.metadata	Logical. Run extract.metadata when importing .asd files and place information in a metadata file? TRUE/FALSE. Default is TRUE
settings.file	settings file used for spectral processing options (OPTIONAL). Contains information related to the spectra collection instrument, output directories, and processing options such as applying a jump correction to the spectra files. Options in the settings file take precedent over options selected in the function call.

Value

output for a single file returns a list with wavelengths and measured reflectance or transmittance values. For a directory, outputs individual ascii text files with wavelength and spectra values for each input ASD file.

Author(s)

Shawn P. Serbin

Examples

```
# Set input file
file.dir <- system.file("extdata/PM01_TIAM_B_LC_REFL00005.asd",package="FieldSpec")
spec <- read.asd(file.dir,out.dir='~',start.wave=350,end.wave=2500,step.size=1)

# Get info from file header
spec <- read.asd(file.dir,out.dir='~')

# Plot output
plot(spec$Wavelength,spec$Spectra,type="l",lwd=2,xlab="Wavelength (nm)", ylab="Reflectance (%)")
```

---

settings *parse settings file used for spectra file import and processing*

Description

Read settings file for spectra import and processing

Usage

```
settings(input.file = NULL)
```

Arguments

input.file	settings file containing information needed for spectra processing

Author(s)

Shawn P. Serbin

Examples

```
## Not run:
settings <- settings()
settings <- settings('/home/$USER/settings.xml')

## End(Not run)
```

`smooth.spectra` *Smooth spectra file with Savitsky-Golay smoothing filter. Works with either a single spectrum or array of spectral observations in row-major format.*

Description

Smooth spectra file with Savitsky-Golay smoothing filter. Works with either a single spectrum or array of spectral observations in row-major format.

Usage

```
smooth.spectra(file.dir = NULL, input.file = NULL,
  out.dir = NULL, out.filename = NULL, header = TRUE,
  p = NULL, n = NULL, length = "full", file.ext = ".csv")
```

Arguments

`file.dir`	Directory of spectra files to apply sgolay smoothing filter.
`input.file`	Spectra file to apply sgolay smoothing filter. If not set then all files in file.dir are processed.
`out.dir`	Output directory for smoothed spectra files. If not set then processed spectra will be output to file.dir
`out.filename`	Output filename for processed spectra file. If not set then the original filename(s) will be modified with the .sg suffix.
`header`	logical. Does the spectra file(s) have a header line? Default = TRUE
`p`	SG filter order. Default 1.
`n`	SG filter length. Needs to be an odd value. Default 21
`length`	Apply sgolay smoothing filter to the entire (default=full) or subset of the spectrum. Define subset limits as (wavelength1,wavelength2), e.g. (2000,2500) in nanometers [NOT YET IMPLEMENTED]
`file.ext`	File extension for spectra files. Default '.csv'

Author(s)

Shawn P. Serbin

Examples

```
## Not run:
smooth.spectra()
smooth.spectra(file.dir=file.dir,input.file=input.file,out.dir=out.dir,out.filename=out.filename,
               header=TRUE,p=1,n=21,length=full)

## End(Not run)
```

`transpose.spectra` *Transpose spectra file(s) from/to row or column major format. Works with either a single spectrum or directory of spectral observations.*

Description

Transpose spectra file(s) from/to row or column major format. Works with either a single spectrum or directory of spectral observations.

Usage

```
transpose.spectra(file.dir = NULL, input.file = NULL,
  out.dir = NULL, out.filename = NULL,
  in.file.ext = ".csv", out.file.ext = ".csv",
  header = FALSE)
```

Arguments

`file.dir`	directory of spectra files to process
`input.file`	name of input spectra file. If ommitted then the function transposes all files in the input file.dir
`out.dir`	output directory for transposed spectra file(s)
`out.filename`	output filename of transposed spectra file(s). If using a directory then the original filenames are appended with the .t suffix
`in.file.ext`	file extension for individual spectra files. Defaults to ".csv"
`out.file.ext`	option to set the output extension. Defaults to ".csv"
`header`	logical. Do/does the file(s) have a header line?

Author(s)

Shawn P. Serbin

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