photobiology Version 0.9.0 User Guide

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December 13, 2015

Contents

1	Intr	roduction	3
2	Inst	allation and use	4
3	Spe	ctra	4
	3.1	print()	4
	3.2	summary()	4
	3.3	Classes	5
	3.4	Data assumptions	5
	3.5	Querying the class	7
	3.6	Construction	8
	3.7	Special attributes	10
4	Col	lections of spectra	13
	4.1	Classes	13
	4.2		14
		4.2.1 Constructors	14
		4.2.2 Using 'as' functions	15
		<u> </u>	15
			16
	4.3	g v	17
	4.4		18
	4.5	· · ·	22
	4.6		25
	4.7		28
5	Way	vebands	29
	5.1	Construction	29
	5.2		30
	5.3	- • •	31

6	Coll	ections of wavebands	31
	6.1	Construction	31
		6.1.1 List constructor	31
		6.1.2 Special constructor	31
7		nsformations: using operators	34
	7.1	Binary operators	34
	7.2	Unary operators and maths functions	38
	7.3	Options	39
8	Trai	nsformations: methods and functions	41
	8.1	Manipulating spectra	41
	8.2	Conversions between radiation units	45
	8.3	Normalizing a spectrum	46
	8.4	Rescaling a spectrum	47
	8.5	Shifting the zero of the spectral data scale	47
	8.6	Replacing off-range spectral data values	48
	8.7	Wavelength interpolation	49
	8.8	Trimming and clipping	49
		8.8.1 Method clip_wl()	49
		8.8.2 Method trim_wl()	51
		8.8.3 Functions trim_spct and trim_spct	53
	8.9	Convolving weights	53
		8.9.1 Individual spectra	53
		8.9.2 Vectors	54
	8.10	Tagging with bands and colours	54
		8.10.1 Individual spectra	54
9	C	nmaries	55
9			55
	9.1 9.2	Summary	58
	9.2	Wavelength	58
		1	58
	9.3	±	59
	9.5	Peaks and valleys	59 59
	0.4	1	61
	9.4	Irradiance	62
		9.4.1 Individual spectra	
		9.4.2 Collections of spectra	63
	0.5	9.4.3 Numeric vectors	65
	9.5	Fluence	65
	0.0	9.5.1 Individual spectra	65 66
	9.6	Photon and energy ratios	66 66
		9.6.1 Individual spectra	66
		9.6.2 Collections of spectra	67
		9.6.3 Vectors	67

	9.7	Normalized difference indexes	68						
	9.8	Individual spectra	68						
	9.9	Transmittance, reflectance, absorptance and absorbance	68						
		9.9.1 Individual spectra	68						
		9.9.2 Collections of spectra	69						
	9.10	Integrated response	69						
		9.10.1 Individual spectra	69						
		9.10.2 Collections of spectra	70						
	9.11	Integration over wavelengths	70						
		9.11.1 Calculation from individual spectra	70						
10	Astr	conomy	70						
	10.1	Position of the sun	70						
	10.2	Times of sunrise, solar noon and sunset $\dots \dots \dots \dots$	72						
11	11 RGB colours								
12	Opti	imizing performance	7 6						
13	Exa	mple data	77						

1 Introduction

We have developed a set of packages to facilitate the calculation of many different quantities that can be derived from spectral irradiance data. The base package in this suite is called photobiology, and is the package described here. There other specialized packages for quantification of ultraviolet radiation and visible radiation (photobiologyWavebands), or plant photoreceptors (photobiologyPlants). Other packages in the suite provide example spectral data for filters (photobiologyFilters), lamps (photobiologyLamps), LEDs (photobiologyLeDs), sunlight (photobiologySun) and broadband sensors (photobiologySensors). In the future it will be submitted to CRAN (Comprehensive R archive network), it is meanwhile available from https://www.r4photobiology.info/. There is also a public Git repository at https://bitbucket.org/aphalo/ from where the source code of the current an earlier versions can be cloned.

Package photobiology provides two sets of functions for many operations: functions programmed following a functional paradigm, and functions using an object-oriented paradigm. The former functions take as arguments numeric vectors and are probably faster. The later ones take 'spectra' objects as arguments, are easier to use, and at least at the moment, to some extent slower. For everyday use 'spectra' objects are recommended, but when maximum performance or flexibility in scripts is desired, the use of the functions taking numeric vectors as arguments may allow optimizations that are not possible with the object-oriented higher level functions.

2 Installation and use

The functions in the package photobiology are made available by installing the packages photobiology (once) and loading it from the library when needed.

To load the package into the workspace we use library(photobiology).

```
library(photobiology)
library(lubridate)
```

3 Spectra

This package defines a family of classes based on data frames which impose some restrictions on the naming of the vectors, something that allows methods and some functions to 'find' the data when passed one of these objects as argument. In addition, as the data is checked when the object is built, there is no need to test for the validity of the data each time a calculation is carried out. The other advantage of using spct objects, is that specialized versions of generic functions like print and operators like + can be defined for spectra. ___spct objects are data.frame objects, as a result of how classes have been derived. In this package we define a generic or base spectrum class, derived from data.frame, from which specialized types of spectra are in turn derived. This 'parenthood' hierarchy means that spectra objects can be used almost anywhere where a data.frame is expected.

3.1 print()

The print() method for spectra is based in the current version of the package on the function defined in package dplyr, consequently, it is possible to the options from this package to control printing. dplyr.print_max, the number of rows in the spectral object above which only dplyr.print_min rows are printed, are both set to 5, instead of the default 20 and 10.

```
options(dplyr.print_max = 4)
options(dplyr.print_min = 4)
```

For explicit calls to print() its argument n can be used to control the number of lines printed. If n is set to Inf the whole spectrum is always printed.

```
print(sun.spct, n = 3)
```

3.2 summary()

The summary() method for spectra is based on base R's summary() method for data frames, and accepts the same arguments, and obeys R's global digits option for its default.

Table 1: Classes for spectral data. In addition to the attributes listed, all spectral objects have attributes normalized and scaled, plus the normal attributes of data.frame objects.

Name	Variables	Attributes
generic_spct raw_spct cps_spct source_spct filter_spct	<pre>w.length w.length, counts w.length, cps w.length, s.e.irrad, s.q.irrad w.length, Tfr, A</pre>	time.unit, bswf Tfr.type
reflector_spct object_spct response_spct chroma_spct	<pre>w.length, Rfr w.length, Tfr, Rfr w.length, s.e.response, s.q.response w.length, x, y, z</pre>	Rfr.type Tfr.type, Rfr.type time.unit

summary(sun.spct)

3.3 Classes

The package defines several classes intended to be used to store different types of spectral data. They are all derived from <code>generic_spct</code>, which in turn is derived from <code>data.frame</code> and internally created using <code>dplyr::data_frame</code>. Table 1 lists them. Attributes are used in objects of these classes to keep <code>metadata</code> such as information about units of expression.

The design imposes that data from different observations are never present as different data columns, if present, additional data columns represent different properties from the same observation event. In most cases, one spectral object corresponds to one spectral observation, but some functions are compatible or can be used to create spectral objects where the spectral data from different observations are stored "longitudinally" and "tagged" with a factor with a level for each observation event. These observations must use consistent units of expression and attribute values.

3.4 Data assumptions

An assumption of the package is that wavelengths are always expressed in nanometres (1 nm = $1 \cdot 10^{-9}$ m). If the data to be analysed uses different units for wavelengths, e.g. Ångstrom (1 Å = $1 \cdot 10^{-10}$ m), the values need to be re-scaled before any calculations. Table 2 lists the units of expression for the different variables listed in Table 1.

Energy irradiances are assumed to be expressed in $W\,m^{-2}$ and photon irradiances in $mol\,m^{-2}\,s^{-1}$, that is to say using second as unit for time. This is the default, but it is possible to set the unit for time to day in the case of source_spct objects.

The default time unit used is second, but day and exposure can be used by

Table 2: Variables used for spectral data and their units of expression: A: as stored in objects of the spectral classes, B: also recognized by the set family of functions for spectra and automatically converted. time.unit accepts in addition to the character strings listed in the table, objects of classes lubridate::duration and period, in addition numeric values are interpreted as seconds. exposure.time accepts these same values, but not the character strings.

Variables	Unit of expression	Attribute value
A: stored		
w.length counts cps s.e.irrad s.e.irrad s.e.irrad s.q.irrad s.q.irrad s.q.irrad ffr Tfr Tfr A Rfr Rfr s.e.response s.e.response s.e.response s.e.response s.q.response s.q.response s.q.response s.q.response s.q.response s.q.response s.q.response s.q.response	$\begin{array}{l} \text{nm} \\ \text{n} \\ \text{n} \\ \text{s}^{-1} \\ \text{W} \\ \text{m}^{-2} \\ \text{nm}^{-1} \\ \text{J} \\ \text{m}^{-2} \\ \text{d}^{-1} \\ \text{nm}^{-1} \\ \text{varies} \\ \text{mol} \\ \text{m}^{-2} \\ \text{s}^{-1} \\ \text{nm}^{-1} \\ \text{mol} \\ \text{m}^{-2} \\ \text{d}^{-1} \\ \text{nm}^{-1} \\ \text{mol} \\ \text{m}^{-2} \\ \text{nm}^{-1} \\ \text{varies} \\ [0,1] \\ [0,1] \\ \text{a.u.} \\ [0,1] \\ [0,1] \\ x \\ \text{J}^{-1} \\ \text{s}^{-1} \\ \text{nm}^{-1} \\ x \\ \text{J}^{-1} \\ \text{d}^{-1} \\ \text{nm}^{-1} \\ x \\ \text{J}^{-1} \\ \text{nm}^{-1} \\ \text{varies} \\ x \\ \text{mol}^{-1} \\ \text{d}^{-1} \\ \text{nm}^{-1} \\ x \\ \text{mol}^{-1} \\ \text{d}^{-1} \\ \text{nm}^{-1} \\ x \\ \text{mol}^{-1} \\ \text{nm}^{-1} \\ \text{mol}^{-1} \\ $	time.unit = "second" time.unit = "day" time.unit = duration time.unit = "second" time.unit = "exposure" time.unit = duration Tfr.type = "total" Tfr.type = "internal" Rfr.type = "specular" time.unit = "second" time.unit = "day" time.unit = "day" time.unit = "exposure" time.unit = "day" time.unit = "second" time.unit = "day" time.unit = "second" time.unit = "day"
B: converted		
$\begin{array}{c} \mathtt{wl} \to \mathtt{w.length} \\ \mathtt{wavelength} \to \mathtt{w.length} \\ \mathtt{Tpc} \to \mathtt{Tfr} \\ \mathtt{Tpc} \to \mathtt{Tfr} \\ \mathtt{Rpc} \to \mathtt{Rfr} \\ \mathtt{Rpc} \to \mathtt{Rfr} \\ \mathtt{Rpc} \to \mathtt{Rfr} \\ \mathtt{counts.per.second} \to \mathtt{cps} \end{array}$	nm nm [0,100] [0,100] [0,100] [0,100] $n \text{s}^{-1}$	Tfr.type = "total" Tfr.type = "internal" Rfr.type = "total" Rfr.type = "specular"

supplying the arguments "day" or "exposure" to a parameter of the constructor of source_spct objects.

The attributes are normally set when an object spectral object is created, either using default values of values supplied as arguments to the constructor.

Not respecting these assumptions will yield completely wrong results! It is extremely important to make sure that the wavelengths are in nanometres as this is what all functions expect. If wavelength values are in the wrong units, the action-spectra weights and quantum conversions will be wrongly calculated, and the values returned by most functions completely wrong, without warning.

If spectral irradiance data is in $\mathrm{W}\,\mathrm{m}^{-2}\,\mathrm{nm}^{-1}$, and the wavelength in nm, as is the case for many Macam spectroradiometers, the data can be used directly and functions in the package will return irradiances in $\mathrm{W}\,\mathrm{m}^{-2}$.

If, for example, the spectral irradiance data output by a spectroradiometer is expressed in $mW\,m^{-2}\,nm^{-1}$, and the wavelengths are in Ångstrom then to obtain correct results when using any of the packages in the suite, we need to rescale the data when creating a new object.

```
# not run
my.spct <- source_spct(w.length = wavelength/10, s.e.irrad = irrad/1000)</pre>
```

In the example above, we take advantage of the behaviour of the S language: an operation between a scalar and vector, is equivalent to applying this operation to each member of the vector. Consequently, in the code above, each value from the vector of wavelengths is divided by 10, and each value in the vector of spectral irradiances is divided by 1000.

3.5 Querying the class

Before giving examples of how to construct objects to store spectral data we show how to query the class of an object, and how to query the class of a spectrum. Consistently with R design, the package provides 'is' functions for querying the type of spectra objects.

```
is.any_spct(sun.spct)
is.source_spct(sun.spct)
```

In addition function class.spc returns directly the spectrum-related class attributes.

```
class_spct(sun.spct)
class(sun.spct)
```

¹The meaning of "exposure" is the total exposure time, in other words, fluence instead of irradiance.

3.6 Construction

There are basically two different approaches to the creation of spectra by users, a constructor similar to data.frame constructor that takes vectors as arguments, and a constructor that converts list objects into spectral objects, which works similarly to as.data.frame from base R. In contrast to the data frame constructors spectral constructor require the variables or the vector arguments should be suitably named so that they can be recognized.

Here we briefly describe the 'as' constructor functions for spectra. In the first example we create an object to store spectral irradiance data for 'light source', by first creting a data frame, and creating the spectral object as a copy of it. In the example below we supply a single value, 1, for the spectral irradiance. This value gets recycled as is normal in R, but of course in real use it is more usual to supply a vector of the same length as the w.length vector.

```
my.df <- data.frame(w.length = 400:410, s.e.irrad = 1)</pre>
my.spct <- as.source_spct(my.df)</pre>
class(my.spct)
## [1] "source_spct" "generic_spct" "tbl_df"
                                                      "tbl"
## [5] "data.frame"
class(my.df)
## [1] "data.frame"
my.spct
## Object: source_spct [11 x 2]
## Wavelength (nm): range 400 to 410, step 1
## Time unit: 1s
##
##
      w.length s.e.irrad
##
         (int)
                  (dbl)
## 1
           400
                       1
## 2
           401
## 3
           402
                        1
## 4
           403
```

We can make a 'generic_spct' copy of any spectrum object.

```
my.g.spct <- as.generic_spct(my.spct)
class(my.g.spct)

## [1] "generic_spct" "tbl_df" "tbl" "data.frame"</pre>
```

When cronstructing spectral objets from numeric vectors the names of the arguments are meaningful and convey information on the nature of the spectral data and basis of expression.

```
source_spct(w.length = 300:305, s.e.irrad = 1)
## Object: source_spct [6 x 2]
## Wavelength (nm): range 300 to 305, step 1
## Time unit: 1s
##
##
   w.length s.e.irrad
##
      (int) (dbl)
## 1
         300
## 2
         301
                    1
## 3
         302
                   1
         303
## 4
                    1
## ..
```

```
z <- 300:305
y <- 2
source_spct(w.length = z, s.e.irrad = y)
## Object: source_spct [6 x 2]
## Wavelength (nm): range 300 to 305, step 1
## Time unit: 1s
##
##
    w.length s.e.irrad
      (int) (dbl)
##
## 1
          300
## 2
                      2
          301
## 3
          302
                    2
## 4
          303
                      2
## ..
```

```
w.length <- 300:305
s.e.irrad <- 1
source_spct(w.length, s.e.irrad)
## Object: source_spct [6 x 2]
## Wavelength (nm): range 300 to 305, step 1
## Time unit: 1s
##
##
    w.length s.e.irrad
##
      (int) (dbl)
## 1
         300
                1
## 2
          301
                     1
## 3
                   1
         302
## 4
          303
## ..
```

The different constructors have additional arguments to be used in setting non-default values for the attributes. These arguments have the same name as the attributes. Here we used the data frame created in the first chunk of the section.

```
my.d.spct <- as.source_spct(my.df, time.unit = "day")</pre>
```

Argument strict.range can be used to override or make more strict the validation of the data values.

```
source_spct(w.length = 300:305, s.e.irrad = -1)
## Warning in range_check(x, strict.range = strict.range): Negative spectral
energy irradiance values; minimun s.e.irrad = -1
## Object: source_spct [6 x 2]
## Wavelength (nm): range 300 to 305, step 1
## Time unit: 1s
##
##
      w.length s.e.irrad
##
         (int)
                   (dbl)
## 1
           300
                      -1
                      -1
## 2
           301
## 3
           302
                      -1
## 4
           303
## ..
source_spct(w.length = 300:305, s.e.irrad = -1, strict.range = NULL)
## Object: source_spct [6 x 2]
## Wavelength (nm): range 300 to 305, step 1
## Time unit: 1s
##
##
      w.length s.e.irrad
##
         (int)
                  (dbl)
## 1
           300
                      -1
## 2
           301
                      -1
## 3
           302
                      -1
## 4
           303
                      -1
## ..
```

Finally argument comment can be used to add a comment to the data at the time of construction.

3.7 Special attributes

Spectral objects have several attributes used to store metadata, such as the time unit used or type of spectral quantity. Some attributes are meaningful for all the classes of spectra defined in the package. These are time of measurement using attribute "when.measured", place of measurement using attribute "where.measured" and free-text comments. One can set and get comments stored in spectra by means of base R's comment() and comment() <- functions. Some of the functions in this package append additional information to comments or merge comments.

Functions setWhenMeasured() and getWhenMeasured() are used for setting or getting a date as a POSIXct value. This format is compatible with many functions from pacakge lubridate.

```
my.spct <- sun.spct
setWhenMeasured(my.spct, NULL)
getWhenMeasured(my.spct)

## [1] NA

setWhenMeasured(my.spct, ymd_hms("2015-10-31 22:55:00", tz = "EET"))
getWhenMeasured(my.spct)

## [1] "2015-10-31 20:55:00 UTC"</pre>
```

Functions setWhereMeasured() and getWhereMeasured() are used for setting or getting a geocode as a data.frame value. This format is comaptible with function geocode() from pacakge ggmap. It is also possible, to simply pass latitude and longitude coordinates, as shown below. The returned value is always a data frame with columns "lon" and "lat".

```
setWhereMeasured(my.spct, NULL)
getWhereMeasured(my.spct)
   lon lat
## 1 NA NA
setWhereMeasured(my.spct, lat = 60, lon = -10)
getWhereMeasured(my.spct)
   lon lat
## 1 -10 60
getWhereMeasured(my.spct)$lon
## [1] -10
my.spct
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2015-10-31 20:55:00 UTC
## Measured at: 60 N, -10 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
      (dbl) (dbl) (dbl)
## 1 280.0000
                 0
                           0
## 2 280.9231
                    0
                              0
## 3 281.8462
                    0
                              0
## 4 282.7692
                    0
                              0
```

Similar functions exist for other attributes which are not shared by all spectral classes. Spectral objects may have several other attributes used to store metadata, such as the time unit used. There functions available for quering and setting the state if these attributes. is_ functions return a logical value, and get functions return the values of the attributes themselves. In addition set

functions can be used to set the value attributes, but many of the set functions are very rarely needed in user code.

The attributes described below are set automatically, and consequently function setBSWFUsed() and other *set* functions for these attributes are mainly of use to programmers extending the package. One exception is when a wrong value has been assigned by mistake and needs to be overwritten.

For example function is_effective() returns TRUE if the spectral data has been weighted with a BSWF. The corresponding getBSWFUsed() function can be used, in this case to retrieve the name of the BSWF that was used when generating the data. Here we demonstrate with one example, where we use two different waveband objects—constructed on-the-fly with constructor functions defined in package photobiologyWavebands—, one defining a range of wavelengths, and another one defining the spectral weighting function for human erythema.

```
is_effective(sun.spct)
## [1] FALSE
is_effective(sun.spct * VIS())
## Error in is_effective(sum.spct * VIS()): could not find function "VIS"
getBSWFUsed(sun.spct * VIS())
## Error in is.source_spct(x): could not find function "VIS"
is_effective(sun.spct * CIE())
## Error in is_effective(sun.spct * CIE()): could not find function "CIE"
getBSWFUsed(sun.spct * CIE())
## Error in is.source_spct(x): could not find function "CIE"
```

Sometimes it may be desired to change the time unit used for expresing spectral irradiance or spectral response, and this can be achieved with the *conversion* function convertTimeUnit. This function both converts spectral data to the new unit of expression and sets the time.unit attribute, preserving the validity of the data object.

```
ten.minutes.spct <-
 convertTimeUnit(sun.spct, time.unit = duration(10, "minutes"))
ten.minutes.spct
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 600s (~10 minutes)
##
##
     w.length s.e.irrad s.q.irrad
               (dbl)
                          (dbl)
##
       (dbl)
## 1 280.0000
                 0
```

Table 3: Classes for collections of spectral objects. Objects of class <code>generic_mspct</code> can have member objects of any class derived from <code>generic_spct</code> and can be heterogeneous. Atributes can be queried and set with the normal R methods of the same names.

Name	Member objects	Attributes		
generic_mspct	<pre>generic_spct + any derived</pre>	names, dim, comment		
raw_mspct	raw_spct	names, dim, comment		
cps_mspct	cps_spct	names, dim, comment		
source_mspct	source_spct	names, dim, comment		
filter_mspct	${ t filter_spct}$	names, dim, comment		
reflector_mspct	$reflector_spct$	names, dim, comment		
object_mspct	object_spct	names, dim, comment		
response_mspct	response_spct	names, dim, comment		
chroma_mspct	chroma_spct	names, dim, comment		

```
## 2 280.9231 0 0
## 3 281.8462 0 0
## 4 282.7692 0 0
## .. ...

getTimeUnit(ten.minutes.spct)
## [1] "600s (~10 minutes)"
```

Spectral objects created with earlier (pre-release) versions of this package are missing some attributes. For this reason 'summary' and 'plot' functions may not work as expected with them. These *old* objects can be updated by adding the missing attribute using functions <code>setTimeUnit</code>, <code>setBSWFUsed</code>, <code>setTfrType</code> and <code>setRfrType</code>. However, in many cases function <code>update_spct</code> can be used to set the missing attributes to default values, or the scripts re-run to rebuild the data objects from raw data.

4 Collections of spectra

4.1 Classes

The package defines several classes intended to be used to store *collections* of different types of spectral data. They are all derived from generic_mspct, which in turn is derived from list. Table 3 lists them.

Objects of these classes, except for those of class <code>generic_mspct</code>, can contain members belonging to one of the classes. Being all other spectral object classes derived from <code>generic_spct</code>, <code>generic_mspct</code> objects can contain heterogeneous collections of spectra. In all cases, there are no restrictions on the lengths, wavelength range and/or wavelength step size, or attributes other than <code>class</code>

of the contained spectra. Mimicking R's arrays and matrixes, a dim attribute is always present and dim methods are provided. These allows the storage of time series of spectral data, or (hyper)spectral image data, or even higher dimensional spectral data. The handling of 1D and 2D spectral collections is already implemented in the summary methods. Handling of 3D and higher dimensional data can be implemented in the future without changing the class definition. By having implemented dim, also methods ncol and nrow are available as they use dim internally. Array-like subscripting is not implemented.

4.2 Construction

4.2.1 Constructors

We can construct a collection using a list of spectral objects as a starting point, in this case the spectral transmittance for two glass filters.

```
two_suns.mspct <- source_mspct(list(sun1 = sun.spct, sun2 = sun.spct))</pre>
two_suns.mspct
## Object: source_mspct [2 x 1]
## --- Member: sun1 --
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
## (dbl) (dbl) (dbl)
## 1 280.0000 0 0
## 1 280.0000 0
## 2 280.9231 0
## 3 281.8462 0
## 4 282.7692 0
                                  0
## ..
## --- Member: sun2 ---
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
      w.length s.e.irrad s.q.irrad
       (db1) (db1) (db1)
280.0000 0 0
280.9231 0 0
##
## 1 280.0000
## 2 280.9231
                0
## 3 281.8462
                                  0
## 4 282.7692
                                   0
## ..
           . . .
## --- FND ---
```

We can also create heterogeneous collections, but this reduces the number of methods that can be used on the resulting collection.

```
mixed.mspct <- generic_mspct(list(filter = clear.spct, source = sun.spct))</pre>
```

4.2.2 Using 'as' functions

The as functions for collections of spectra, not only change the class of the collection object, but also apply the corresponding as functions to the member objects. They copy the original objects and then convert the copy, which is returned.

```
two_gen.mscpt <- as.generic_mspct(two_suns.mspct)
class(two_gen.mscpt)

## [1] "generic_mspct" "list"

lapply(two_gen.mscpt, class_spct)

## $sun1

## [1] "source_spct" "generic_spct"

## ## $sun2

## [1] "source_spct" "generic_spct"</pre>
```

4.2.3 Converting 'tidy' data

Spectral objects containing multiple spectra identified by a factor (class of the argument is replicated to collection members).

```
two_suns.spct <- rbindspct(list(a = sun.spct, b = sun.spct / 2))</pre>
subset2mspct(two_suns.spct)
## Object: source_mspct [2 x 1]
## --- Member: a --
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
## (dbl) (dbl) (dbl)
## 1 280.0000 0 0
## 2 280.9231 0 0
## 3 281.8462 0 0
## 4 282.7692 0 0
## ... ... ... ...
## --- Member: b ---
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
##
      w.length s.e.irrad s.q.irrad
## (db1) (db1) (db1)
## 1 280.0000 0 0
## 2 280.9231 0 0
```

```
## 3 281.8462 0 0
## 4 282.7692 0 0
## ... ... ...
```

Data frame containing 'tidy' spectral data (target class and index variable need to be supplied as arguments).

```
test1.df <- data.frame(w.length = rep(200:210, 2),
                     s.e.irrad = rep(c(1, 2), c(11, 11)),
                     spectrum = factor(rep(c("A", "B"), c(11,11))))
subset2mspct(test1.df, member.class = "source_spct", idx.var = "spectrum")
## Object: source_mspct [2 x 1]
## --- Member: A --
## Object: source_spct [11 x 2]
## Wavelength (nm): range 200 to 210, step 1
## Time unit: 1s
##
##
     w.length s.e.irrad
##
      (int) (dbl)
         200 1
201 1
202 1
203
## 1
        200
## 2
                 1
## 3
      203
## 4
## ..
## --- Member: B ---
## Object: source_spct [11 x 2]
## Wavelength (nm): range 200 to 210, step 1
## Time unit: 1s
##
##
     w.length s.e.irrad
##
      (int) (dbl)
                2 2
## 1
         200
## 2
        201
## 3
        202
## 4
        203
## ..
         . . .
## --- END ---
```

4.2.4 Converting 'untidy' data frames

Data frame containing 'untidy' or 'wide' spectral data (class is determined by the function used, columns which are not numeric are skipped.

```
test2.df <- data.frame(w.length = 200:210, A = 1, B = 2, z = "A")
split2source_mspct(test2.df)

## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [11 x 2]
## Wavelength (nm): range 200 to 210, step 1
## Time unit: 1s
##
## w.length s.e.irrad</pre>
```

```
(int) (dbl)
## 1
         200
                 1
## 2
          201
                     1
## 3
          202
                     1
## 4
          203
                   1
## ..
## --- Member: B ---
## Object: source_spct [11 x 2]
## Wavelength (nm): range 200 to 210, step 1
## Time unit: 1s
##
##
     w.length s.e.irrad
##
      (int) (dbl)
                 2
## 1
         200
## 2
         201
## 3
         202
        203
                   2
## 4
## ..
         . . .
## --- END ---
split2source_mspct(test2.df, spct.data.var = "s.q.irrad")
## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [11 x 2]
## Wavelength (nm): range 200 to 210, step 1
## Time unit: 1s
##
##
     w.length s.q.irrad
      (int) (dbl)
##
## 1
        200
                 1
         201
                   1
## 2
## 3
          202
                     1
                  1
## 4
          203
## ..
## --- Member: B ---
## Object: source_spct [11 x 2]
## Wavelength (nm): range 200 to 210, step 1
## Time unit: 1s
##
##
     w.length s.q.irrad
##
      (int) (dbl)
                 2 2
## 1
         200
## 2
          201
## 3
         202
## 4
         203
                     2
## ..
## --- END ---
```

4.3 Querying the class

is. functions are defined for these classes. R's class method can also be used.

```
is.source_mspct(two_suns.mspct)
## [1] TRUE
```

```
class(two_suns.mspct)
## [1] "source_mspct" "generic_mspct" "list"
```

In addition to using class to query the class of the collection, we can use base R's lapply together with class or class_spct to query the class of each of the members of the collection.

```
is.filter_mspct(mixed.mspct)
## [1] FALSE
is.any_mspct(mixed.mspct)
## [1] TRUE
class(mixed.mspct)
## [1] "generic_mspct" "list"
lapply(mixed.mspct, class_spct)
## $filter
## [1] "filter_spct" "generic_spct"
## $source
## [1] "source_spct" "generic_spct"
lapply(mixed.mspct, class)
## $filter
## [1] "filter_spct" "generic_spct" "tbl_df"
                                                    "tbl"
## [5] "data.frame"
##
## $source
## [1] "source_spct" "generic_spct" "tbl_df"
                                                    "tbl"
## [5] "data.frame"
```

4.4 Extract, replace and combine

R's extraction and replacement methods have specializations for collections of spectra and can be used with the same syntax and functionality as for R lists. However they test the class and validity of the returned objects and replacement members.

Methods '[', and '[<-', extract and replace 'parts' of the collection, respectively. Even when only one member is extrated, the returned value is a collection of spectra. The expected replacement value is also, always a collection of spectra.

```
two_suns.mspct[1]
## Object: source_mspct [1 x 1]
## --- Member: sun1 ---
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
    w.length s.e.irrad s.q.irrad
## --- END ---
two_suns.mspct[2:1]
## Object: source_mspct [2 x 1]
## --- Member: sun2 ---
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1 \,
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
    w.length s.e.irrad s.q.irrad
## (dbl) (dbl) (dbl)
## 1 280.0000 0 0
## 2 280.9231 0 0
## 3 281.8462 0 0
## 4 282.7692 0 0
## 4 282.7692
## --- Member: sun1 ---
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
     (dbl) (dbl) (dbl)
##
               (db1) (db1)
0 0
0 0
0 0
0 0
## 1 280.0000
## 2 280.9231
## 3 281.8462
## 4 282.7692
## .. ...
## --- END ---
```

```
two_suns.mspct[1:2] <- two_suns.mspct[2:1]</pre>
```

Methods '[[', \$ and '[[<-', extract and replace individual members of the collection, respectively. They allways return or expect objects of one of the spectral classes.

```
two_suns.mspct[[1]]
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
## (db1) (db1) (db1)
## 1 280.0000 0 0
## 2 280.9231 0 0
## 3 281.8462 0 0
## 4 282.7692 0 0
## .. ...
                      . . .
two_suns.mspct$sun1
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
## 1 280.0000 0 0
## 2 280.9231 0 0
## 3 281.8462 0 0
## 4 282.7692 0 0
##
        (dbl) (dbl) (dbl)
two_suns.mspct[["sun1"]]
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1 \,
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
      w.length s.e.irrad s.q.irrad
##
## (db1) (db1) (db1)
## 1 280.0000 0 0
## 2 280.9231 0 0
## 3 281.8462 0 0
## 4 282.7692 0 0
## .. ...
```

```
two_suns.mspct[["sun1"]] <- sun.spct * 2</pre>
two_suns.mspct[["sun2"]] <- NULL</pre>
two_suns.mspct
## Object: source_mspct [2 x 1]
## --- Member: sun1 --
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1 \,
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
##
      (db1) (db1)
                 0
## 1 280.0000
## 2 280.9231
                    0
## 3 281.8462
## 4 282.7692
                     0
## ..
                    . . .
## --- END ---
```

We can use the combine method c() with collections of spectra (but not to create new collections from individual spectra).

```
c(two_suns.mspct, mixed.mspct)
## Object: generic_mspct [3 x 1]
## --- Member: sun1 ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1 \,
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
    w.length s.e.irrad
      (dbl) (dbl)
##
                0
## 1 280.0000
## 2 280.9231
## 3 281.8462
                   0
## 4 282.7692
                    0
## ..
      . . .
## --- Member: filter ---
## Object: filter_spct [4 x 2]
## Wavelength (nm): range 100 to 5000, step 1 to 4898
##
## w.length Tfr
##
     (dbl) (dbl)
## 1
        100 1
## 2
        101
               1
## 3
        4999
              1
## 4
       5000
## --- Member: source ---
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
```

Table 4: Apply fucntions for collections of spectra. Key: v., value returned by 'apply' function; f.v., value returned by the applied function (argument .fun). In the table generic_mspct and generic_spct indicate objects of these classes or any class derived from them. The exact class of the collection of spectra object returned will be determined by the class(es) of the values returned by the applied function.

'apply' function	first arg. class	v. class	f.v. class	f.v. length	f.v. dims
msmsply msdply mslply msaply msaply concolve_each	generic_mspct generic_mspct generic_mspct generic_mspct generic_mspct generic_mspct	generic_mspct data.frame list vector matrix generic_mspct	generic_spct numeric any any simple any simple generic_spct	$ \begin{array}{c} 1\\ 1 \dots n\\ \text{any}\\ 1\\ 2 \dots n\\ 1 \end{array} $	any 1 any 0 $2 \dots n$ any

```
## Time unit: 1s
##
##
    w.length s.e.irrad s.q.irrad
     (dbl) (dbl) (dbl)
##
              0
## 1 280.0000
                      0
## 2 280.9231
                 0
                         0
## 3 281.8462
                0
                         0
## 4 282.7692
                0
                         0
## .. ...
## --- END ---
```

4.5 Transform or apply functions

For our 'apply' functions we follow the naming convention used in package plyr, but using ms as prefix for _mspct objects. The 'apply' functions implemented in the photobiology package are msmsply, msdply, mslply and msaply which both accepts a collections of spectra as first argument and return a collection of spectra, a data frame, a list, or an array respectively (Table 4).

Functions msmsply(), msdply and mslply can be used to apply a function to each member spectrum in a collection. The 'apply' function to use depends on the return value of the applied function.

In the case of msmsply() the applied function is expected to return a 'transformed' spectrum as another object of class generic_spct or a class derived from it. The value returned by msmsply is a collection of spectra, of a type determined by the class(es) of the member spectra in the new collection.

We start with a simple example in which we add a constant to each spectrum in the collection

```
two.mspct <- source_mspct(list(A = sun.spct * 1, B = sun.spct * 2))
msmsply(two.mspct, `+`, 0.1)

## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC</pre>
```

```
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
     (dbl) (dbl)
              0.1
## 1 280.0000
## 2 280.9231
## 3 281.8462
                  0.1
## 4 282.7692
                  0.1
## .. ...
                   . . .
## --- Member: B ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
##
      (dbl) (dbl)
## 1 280.0000
                 0.1
## 2 280.9231
                  0.1
## 3 281.8462
                  0.1
## 4 282.7692
                  0.1
## .. ...
## --- END ---
```

and continue with a more complex example in which we trim each spectrum

```
msmsply(two.mspct, trim_wl, range = c(281, 500), fill = NA)
## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [525 x 2]
## Wavelength (nm): range 280 to 800, step 1.023182e-12 to 1
## Time unit: 1s
##
## w.length s.e.irrad
##
      (dbl) (dbl)
## 1 280.0000
               NA
NA
## 2 280.9231
## 3 281.0000
## 4 281.0000
                   0
## .. ... ...
## --- Member: B ---
## Object: source_spct [525 x 2]
## Wavelength (nm): range 280 to 800, step 1.023182e-12 to 1
## Time unit: 1s
##
##
     w.length s.e.irrad
##
      (dbl) (dbl)
## 1 280.0000
## 2 280.9231
                   NA
## 3 281.0000
                    NA
                  0
## 4 281.0000
## .. ...
## --- END ---
```

In the second example we pass two arguments by name to the applied function. The number of arguments is not fixed, but the spectrum will be always passed as the first argument to the function.

In the case of msdply() the applied function is expected to return an R object of the same length for each of the member spectra.

In the case of mslply() the applied function is expected to return an R object of any length, possibly variable among members.

```
str(mslply(two.mspct, names))
## List of 2
## $ A: chr [1:2] "w.length" "s.e.irrad"
## $ B: chr [1:2] "w.length" "s.e.irrad"
## - attr(*, "comment") = chr "Applied function: 'names'.\n"
```

In the case of msaply() the applied function is expected to return an R object of length 1, although a list with dimensions will be returned for longer return values.

```
str(msaply(two.mspct, max))
## atomic [1:2] 800 800
## - attr(*, "comment") = chr "Applied function: 'max'.\n"
```

```
str(msaply(two.mspct, range))
## num [1:2, 1:2] 280 280 800 800
## - attr(*, "dimnames")=List of 2
## ..$: NULL
## ..$: chr [1:2] "1" "2"
## - attr(*, "comment")= chr "Applied function: 'range'.\n"
```

4.6 Convolution

By convolution we normally mean the multiplication value by value at matching wavelengths of two spectra. The function described in this section facilitates this and similar operations among collections of spectra. An example use case could be the covolution of spectral irradiance by spectral transmittance for all combinations of light sources and filters in a collection of source spectra and a collection of filter spectra.

Default operator (or function) is that for multiplication, either one or both of the two first arguments must be a collection of spectra. When only one argument is a collection of spectra, the other one can be a spectrum, or even a numeric vector. For multiplication the order of the operands does not affect the returned value. With operators or functions for non-transitive operations the order does matter.

```
convolve_each(two.mspct, sun.spct)
## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
##
    w.length s.e.irrad
##
       (dbl) (dbl)
## 1 280.0000
                     0
## 2 280.9231
                     0
## 3 281.8462
## 4 282.7692
## ..
## --- Member: B ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
##
     w.length s.e.irrad
  (dbl) (dbl)
##
```

```
## 1 280.0000 0

## 2 280.9231 0

## 3 281.8462 0

## 4 282.7692 0

## .. .. ...

## --- END ---
```

```
convolve_each(sun.spct, two.mspct)
## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
## w.length s.e.irrad
##
     (dbl) (dbl)
## 1 280.0000
## .. ...
## --- Member: B ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
## w.length s.e.irrad
## (dbl) (dbl)
                0
## 1 280.0000
                   0
## 2 280.9231
             0
## 3 281.8462
## 4 282.7692
## .. ...
## --- END ---
```

```
another_two.mspct <- two.mspct</pre>
names(another_two.mspct) <- c("a", "b")</pre>
convolve_each(another_two.mspct, two.mspct)
## Object: source_mspct [2 x 2]
## --- Member: a_A ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1 \,
## Time unit: 1s
##
## w.length s.e.irrad
## (dbl) (dbl)
## 1 280.0000
                 0
## 2 280.9231
## 3 281.8462
                 0
## 4 282.7692
## 4 202.1032
## --- Member: a_B ---
## Object: source_spct [522 x 2]
```

```
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
##
     w.length s.e.irrad
## (db1) (db1)
## 1 280.0000 0
## 2 280.9231 0
## 3 281.8462 0
                   0
## 4 282.7692
## .. ...
## --- Member: b_A ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
## w.length s.e.irrad
##
      (dbl) (dbl)
               0
## 1 280.0000
## 2 280.9231
## 3 281.8462
## 4 282.7692
                   0
## .. ...
## --- Member: b_B ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
##
    w.length s.e.irrad
##
      (dbl) (dbl)
## 1 280.0000
## 2 280.9231
                    0
## 3 281.8462
                     0
                   0
## 4 282.7692
## .. ...
## --- END ---
```

The function convolve_each will use other operators or functions and even pass additional named arguments when these are supplied as arguments.

```
convolve_each(two.mspct, sun.spct, oper = `+`)
## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
##
##
    w.length s.e.irrad
##
     (dbl) (dbl)
## 1 280.0000
## 2 280.9231
                   0
## 3 281.8462
                    0
                  0
## 4 282.7692
## .. ...
## --- Member: B ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
```

There are cases where functions convolve_each() and msmsply() can be both used, but there are also cases where their differences matter. An example is convolving two collections of spectra, a case where only convolve_each() can be used. In contrast, when one of the arguments is not a spectrum or a collection of spectra, msmsply() should be used instead.

4.7 Attributes

Some of the set and get functions used with attributes have method definitions for collections of spectra. Some examples follow.

```
getWhenMeasured(two.mspct)
## Source: local data frame [2 x 2]
##
                   when.measured
##
    spct.idx
## (fctr) (time)
## 1 A 2010-06-22 09:51:00
           B 2010-06-22 09:51:00
setWhenMeasured(two.mspct, ymd("2015-10-31"))
getWhenMeasured(two.mspct)
## Source: local data frame [2 x 2]
##
   spct.idx when.measured
     (fctr) (time)
A 2015-10-31
B 2015-10-31
##
## 1
## 2
setWhenMeasured(two.mspct,
     list(ymd_hm("2015-10-31 10:00"),
                     ymd_hm("2015-10-31 11:00")))
getWhenMeasured(two.mspct)
## Source: local data frame [2 x 2]
##
                   when.measured
##
     spct.idx
## (fctr) (time)
## 1 A 2015-10-31 10:00:00
## 2 B 2015-10-31 11:00:00
```

```
two.mspct
## Object: source_mspct [2 x 1]
## --- Member: A ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2015-10-31 10:00:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
      w.length s.e.irrad
##
        (dbl)
                (dbl)
## 1
     280.0000
                      0
## 2 280.9231
                      Ω
## 3 281.8462
## 4 282.7692
                      0
## ..
        . . .
## --- Member: B ---
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2015-10-31 11:00:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
      w.length s.e.irrad
##
       (dbl) (dbl)
## 1 280.0000
## 2 280.9231
                       0
## 3 281.8462
                       0
## 4 282.7692
                       0
## ..
## --- END ---
```

Other methods available are getWhereMeasured and setWhereMeasured.

5 Wavebands

When a range of wavelengths or a range of wavelengths plus a spectral weighting function (SWF) is needed for radiation summaries or transformations, methods, operators and functions defined in package photobiology use waveband objects to store these data. A few other bits of information can be included to fine-tune calculations. The waveband definitions do NOT describe whether input spectral irradiances are photon or energy based, nor whether the output irradiance will be based on photon or energy units. All waveband objects belong to the S3 class waveband.

5.1 Construction

When defining a waveband which uses a SWF, a function can be supplied either based on energy effectiveness, on photon effectiveness, or one function for each one. If only one function is supplied the other one is built automatically, but if performance is a concern it is better to provide two separate functions. Another

case when you might want to enter the same function twice, is if you are using an absorptance spectrum as SWF, as the percent of radiation absorbed will be independent of whether photon or energy units are used for the spectral irradiance.

To create a waveband object we use constructor function waveband, and optionally giving a name to it.

```
PAR <- waveband(c(400, 700), wb.name = "PAR")
UVA <- waveband(c(315, 400), wb.name = "UVA")
UVB <- waveband(c(280, 315), wb.name = "UVB")
UVC <- waveband(c(100, 280), wb.name = "UVC")
UV <- waveband(c(100, 400), wb.name = "UV")
```

When including a BSWF, we supply, one or two versions of functions returning the weights as a function of wavelength. Several such functions are defined in package photobiologyWavebands as well as constructors using them. Here we give three examples of how equivalent wavebands can be defined based on a SWF. Although the constructor is smart enough to derive the missing function when only one function is supplied, performance may suffer.

The first argument to waveband() does not need to be a numeric vector of length two. Any R object of a class that supplies a range() method definition that can be interpreted as a range of wavelengths in nanometres can be used. As a consequence, when wanting to construct a waveband covering the whole range of a spectrum one can simply supply the spectrum as argument, or to construct an unweighted waveband which covers exactly the same range of wavelengths as an existing effective (weighted) waveband, one can supply a waveband object as an argument.

```
waveband(sun.spct)

## Total
## low (nm) 280
## high (nm) 800
## weighted none
```

5.2 Querying the class

The function is.waveband can the used to query any R object. This function returns a logical value.

```
is.waveband(PAR)
## [1] TRUE
```

Above, we demonstrate that PAR is a waveband object, the function photobiologyWavebands::PAR() is a waveband constructor returning a waveband object. See package photobiologyWavebands for details on pre-defined waveband constructors for frequently used wavelength ranges and biological spectral weighting functions (BSWFs).

5.3 Retrieving properties

The function is_effective can the used to query any R object.

```
is_effective(PAR())
## Error in is_effective(PAR()): could not find function "PAR"
```

6 Collections of wavebands

In the current implementation there is no special class used for storing collections of waveband objects. We simply use base R's list class.

6.1 Construction

6.1.1 List constructor

Just base R's functions used to create a list object.

```
wavebands <- list(waveband(c(300,400)), waveband(c(400,500)))
wavebands

## [[1]]
## range.300.400
## low (nm) 300
## high (nm) 400
## weighted none
##

## [[2]]
## range.400.500
## low (nm) 400
## high (nm) 500
## weighted none</pre>
```

6.1.2 Special constructor

The function split_bands can be used to generate lists of unweighted wavebands in two different ways: a) it can be used to split a range of wavelengths

given by an R object into a series of adjacent wavebands, or b) with a list of objects returning ranges, it can be used to create non-adjacent and even overlapping wavebands.

The code chunk bellow shows an example of two variations of case a). With the default value for length.out of NULL each numerical value in the input is taken as a wavelength (nm) at the boundary between adjacent wavebands. If a numerical value is supplied to length.out, then the whole wavelength range of the input is split into this number of equally spaced adjacent wavebands.

```
split_bands(c(200, 225, 300))
## $wb1
## range.200.225
## low (nm) 200
## high (nm) 225
## weighted none
##
## $wb2
## range.225.300
## low (nm) 225
## high (nm) 300
## weighted none
split_bands(c(200, 225, 300), length.out = 2)
## $wb1
## range.200.250
## low (nm) 200
## high (nm) 250
## weighted none
## $wb2
## range.250.300
## low (nm) 250
## high (nm) 300
## weighted none
```

In both examples above, the output is a list of two wavebands, but the 'split' boundaries are at a different wavelength. The chunk bellow gives a few more examples of the use of case a).

```
## $wb1
## range.280.540
## low (nm) 280
## high (nm) 540
## weighted none
##
## $wb2
## range.540.800
## low (nm) 540
## high (nm) 800
## weighted none
```

```
split_bands(PAR(), length.out = 2)
## Error in is.any_spct(x): could not find function "PAR"
split_bands(c(200, 800), length.out = 3)
## $wb1
## range.200.400
## low (nm) 200
## high (nm) 400
## weighted none
##
## $wb2
## range.400.600
## low (nm) 400
## high (nm) 600
## weighted none
##
## $wb3
## range.600.800
## low (nm) 600
## high (nm) 800
## weighted none
```

Now we demonstrate case b). This case is handled by recursion, so each list element can be anything that is a valid input to the function, including a nested list. However, the returned value is always a flat list of wavebands.

```
split_bands(list(A = c(200, 300), B = c(400, 500), C = c(250, 350)))
## $A
## range.200.300
## low (nm) 200
## high (nm) 300
## weighted none
##
## $B
## range.400.500
## low (nm) 400
## high (nm) 500
## weighted none
##
## $C
## range.250.350
## low (nm) 250
## high (nm) 350
## weighted none
split_bands(list(c(100, 150, 200), c(800, 825)))
## $wb.a
## range.100.150
## low (nm) 100
## high (nm) 150
## weighted none
##
```

```
## $<NA>
## range.150.200
## low (nm) 150
## high (nm) 200
## weighted none
##
## $wb.b
## range.800.825
## low (nm) 800
## high (nm) 825
## weighted none
```

In case b) if we supply a numeric value to length.out, this value is used recursively for each element of the list.

```
split_bands(list(R = Red(), B = Blue()), length.out = 2)

## Error in is.any_spct(x): could not find function "Red"

split_bands(list(c(100, 150, 200), c(800, 825)), length.out = 1)

## $wb.a

## range.100.200

## low (nm) 100

## high (nm) 200

## weighted none

##

##

## $wb.b

## range.800.825

## low (nm) 800

## high (nm) 825

## weighted none
```

7 Transformations: using operators

7.1 Binary operators

The basic maths operators have definitions for spectra. It is possible to sum, subtract, multiply and divide spectra. These operators can be used even if the spectral data is on different arbitrary sets of wavelengths. Operators by default use values expressed in energy units. Only certain operations are meaningful for a given combination of objects belonging to different classes, and meaningless combinations return NA also issuing a warning (see Table 5). By default operations are carried out on spectral energy irradiance for source_spct objects and transmittance for filter_spct objects.

```
sun.spct * sun.spct
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Time unit: 1s
```

Table 5: Binary operators and operands. Validity and class of result. All operations marked 'Y' are allowed, those marked 'N' are forbidden and return NA and issue a warning. Operators % and % follow /.

e1	+	-	*	/	^	e2	value
raw_spct	Y	Y	Y	Y	Y	raw_spct	raw_spct
cps_spct	Y	Y	Y	Y	\mathbf{Y}	cps_spct	cps_spct
source_spct	Y	Y	Y	Y	\mathbf{Y}	source_spct	source_spct
filter_spct (T)	N	N	Y	Y	N	$filter_spct$	$filter_spct$
filter_spct (A)	Y	Y	N	N	N	$filter_spct$	$filter_spct$
reflector_spct	N	N	Y	Y	N	$reflector_spct$	reflector_spct
object_spct	N	N	N	N	N	object_spct	
response_spct	Y	Y	Y	Y	N	response_spct	response_spct
${\tt chroma_spct}$	Y	Y	Y	Y	Y	chroma_spct	${\tt chroma_spct}$
raw_spct	Y	Y	Y	Y	Y	numeric	raw_spct
cps_spct	\mathbf{Y}	\mathbf{Y}	Y	\mathbf{Y}	\mathbf{Y}	numeric	cps_spct
source_spct	Y	Y	Y	Y	Y	numeric	source_spct
filter_spct	Y	Y	Y	Y	Y	numeric	filter_spct
reflector_spct	Y	Y	Y	Y	Y	numeric	reflector_spct
object_spct	N	N	N	N	N	numeric	
response_spct	Y	Y	Y	Y	\mathbf{Y}	numeric	response_spct
chroma_spct	Y	Y	Y	Y	Y	numeric	chroma_spct
source_spct	N	N	Y	Y	N	response_spct	response_spct
source_spct	N	N	\mathbf{Y}	Y	N	filter_spct (T)	source_spct
source_spct	N	N	Y	\mathbf{Y}	N	filter_spct (A)	source_spct
source_spct	N	N	Y	\mathbf{Y}	N	reflector_spct	source_spct
source_spct	N	N	N	N	N	object_spct	
source_spct	N	N	Y	N	N	waveband (no BSWF)	source_spct
source_spct	N	N	Y	N	N	waveband (BSWF)	source_spct

When meaningful, operations between different spectra are also allowed. For example, it is possible to simulate the effect of a filter on a light source by multiplying (or convolving) the two spectra.

If we have two layers of the filter, this can be approximated using either of these two statements.

```
sun.spct * polyester.spct * polyester.spct
## Object: source_spct [533 x 2]
## Wavelength (nm): range 280 to 800, step 0.07692308 to 1
## Time unit: 1s
##
##
   w.length s.e.irrad
##
      (dbl) (dbl)
## 1 280.0000
              0
## 2 280.9231
                   0
## 3 281.0000
                  0
                 0
## 4 281.8462
## ..
sun.spct * polyester.spct^2
## Object: source_spct [533 x 2]
## Wavelength (nm): range 280 to 800, step 0.07692308 to 1 \,
## Time unit: 1s
##
##
    w.length s.e.irrad
##
     (dbl) (dbl)
## 1 280.0000
               0
## 2 280.9231
                   0
## 3 281.0000
                  0
```

Operators are also defined for operations between a spectrum and a numeric vector (with normal recycling).

```
sun.spct * 2
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
##
       (dbl) (dbl)
## 1 280.0000
                0
## 2 280.9231
## 3 281.8462
                   0
## 4 282.7692
                   0
## .. ...
                  . . .
2 * sun.spct
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
    w.length s.e.irrad
##
##
      (dbl) (dbl)
                0
## 1 280.0000
## 2 280.9231
## 3 281.8462
                   0
## 4 282.7692
## ..
sun.spct * c(0,1)
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
##
     (dbl) (dbl)
                0
## 1 280.0000
## 2 280.9231
                   0
## 3 281.8462
                    0
## 4 282.7692
                    0
## ..
```

There is one special case, for chroma_spct: if the numeric operand has length three, containing three *named* values 'x', 'y' and 'z', the corresponding value is used for each of the chromaticity 'columns' in the chroma_spct. Un-named values or differently named values are not treated specially.

Operators are also defined for operations between an spectrum and a

Table 6: Unary operators and maths functions for spectra. Classes for which they are implemented and class of the result. All operations marked 'Y' are allowed, those marked 'N' are not implemented and return NA and issue a warning. Additional supported functions: log2, log10, sin, cos, tan, asin, acos, atan, sinpi, cospi, tanpi, signif, floor, ceiling, trunc, sign, abs.

e1	+, -	log, exp	trig.	round	sqrt	value
raw_spct	Y	Y	Y	Y	Y	raw_spct
cps_spct	Y	Y	Y	Y	Y	cps_spct
source_spct	Y	Y	Y	Y	Y	source_spct
filter_spct	Y	Y	Y	Y	Y	filter_spct
reflector_spct	Y	Y	Y	Y	Y	reflector_spct
object_spct	N	N	N	N	N	
response_spct	\mathbf{Y}	\mathbf{Y}	\mathbf{Y}	Y	\mathbf{Y}	response_spct
chroma_spct	\mathbf{Y}	\mathbf{Y}	Y	Y	Y	chroma_spct

waveband object. The next to code chunks demonstrate how the class of the result depends on whether the waveband object describes a range of wavelengths or a range of wavelengths plus a BSWF.

```
sun.spct * UVB()
## Error in eval(expr, envir, enclos): could not find function "UVB"
sun.spct * CIE()
```

Error in eval(expr, envir, enclos): could not find function "CIE"

And of course these operations can be combined into more complex statements, including parentheses, when needed. The example below estimates the difference in effective spectral irradiance according to the CIE98 definition, between sunlight and sunlight filtered with a polyester film. Of course, the result is valid only for the solar spectral data used, which corresponds to Southern Finland.

```
sum.spct * CIE() - sum.spct * polyester.spct * CIE()
## Error in eval(expr, envir, enclos): could not find function "CIE"
```

7.2 Unary operators and maths functions

The most common maths functions, as well as unary minus and plus, are also implemented for spectral objects (see Table 6).

```
-sun.spct

## Object: source_spct [522 x 2]

## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
```

```
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
##
       (dbl) (dbl)
## 1 280.0000
## 2 280.9231
                     0
## 3 281.8462
                    0
## 4 282.7692
## ..
sqrt(sun.spct)
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
##
       (dbl) (dbl)
## 1 280.0000
## 2 280.9231
                     0
## 3 281.8462
                     0
## 4 282.7692
                      0
```

7.3 Options

Table 7 lists all the recognized options affecting maths operators and functions, and their default values. Within the suite all functions have a default value which is used when the options are undefined. Options are set using base R's function options, and queried with functions options and getOption.

The behaviour of the operators defined in this package depends on the value of two global options. For example, if we would like the operators to operate on spectral photon irradiance and return spectral photon irradiance instead of spectral energy irradiance, this behaviour can be set, and will remain active until unset or reset.

```
options(photobiology.radiation.unit = "photon")
sun.spct * UVB()

## Error in eval(expr, envir, enclos): could not find function "UVB"

options(photobiology.radiation.unit = "energy")
sun.spct * UVB()

## Error in eval(expr, envir, enclos): could not find function "UVB"
```

The other options listed in Table 7 can be set similarly, to unset any option, they can be given a NULL value.

Table 7: Options recognized by functions in the photobiology package and the values they can take.

Option	values, <u>default</u>	function
Base R		
digits	7	d-3 used by summary
photobiology.radiation.unit	"energy" "photon"	output $(W m^{-2} nm^{-1})$ output $(mol m^{-2} s^{-1} nm^{-1})$
photobiology.filter.qty	"transmittance" "absorptance" "absorbance"	output $(/1)$ output $(/1)$ output $(a.u. \log_{10} base)$
photobiology.use.hinges	<u>NULL</u> TRUE FALSE	guess automatically do not insert hinges do insert hinges
photobiology.strict.range	NA TRUE <u>FALSE</u>	skip range test trigger and error trigger a warning
photobiology. auto. hinges. limit	0.5	wavelength step (nm)
photobiology. waveband. trim	FALSE TRUE	exclude trim or exclude
photobiology.use.cached.mult	FALSE TRUE	do not cache intermediate results cache intermediate results
photobiology.verbose	FALSE TRUE	do not give verbose output give verbose output

Table 8: Transformation methods for spectra. Key: + available, - not available, f available in the future.

methods	source	response	filter	reflector	object	chroma
merge	+	+	+	+	+	+
rbindspct	+	+	+	+	+	+
e2q, q2e	+	+	_	-	_	_
A2T, T2A	_	-	+	_	-	_
subset	+	+	+	+	+	+
clip_wl	+	+	+	+	+	+
trim_wl	+	+	+	+	+	+
(trim_spct)	+	+	+	+	+	+
$interpolate_wl$	+	+	+	+	+	+
$(interpolate_spct)$	+	+	+	+	+	+
fscale	+	+	+	+	_	_
fshift	+	+	+	+	_	_
normalize	+	+	+	+	_	_
clean	+	+	+	+	-	_
math operators	+	+	+	+	+	+
math functions	+	+	+	+	+	+
tag	+	+	+	+	+	+
untag	+	+	+	+	+	+

8 Transformations: methods and functions

In this section we describe methods and functions that take one or more spectral objects, and in some cases also waveband objects, as arguments and return another spectral object (Table 8) or that take a collection of spectral objects, and in some cases also waveband objects, as arguments and return a collection of spectral objects (Table 9).

8.1 Manipulating spectra

Sometimes, especially for plotting, we may want to row-bind spectra. When the aim is that the returned object retains its class and other attributes like the time unit. Package photobiology provides function rbinspct for row-binding spectra, with the necessary checks for consistency of the bound spectra.

```
# STOPGAP
shade.spct <- sun.spct</pre>
```

By default an ID factor named spct.idx is added allow to idetify the source of the observations after the binding. If the supplied list has named members, then these names are used as factor levels. If a character value is supplied to as idfactor argument, this is used as name for the factor.

```
rbindspct(list(sun.spct, shade.spct))
## Object: source_spct [1,044 x 4]
## Wavelength (nm): range 280 to 800, step -520 to 1
```

Table 9: Transformation methods for collections of spectra. Key: + available, - not available, ms use msmsply() or $convolve_each()$ to apply function or operator to collection members.

methods	source	response	filter	reflector	object	chroma
${\tt convolve_each}$	+	+	+	+	+	+
msmsply	+	+	+	+	+	+
msdply	+	+	+	+	+	+
mslply	+	+	+	+	+	+
msaply	+	+	+	+	+	+
rbindspct	+	+	+	+	+	+
С	+	+	+	+	+	+
math operators	ms	ms	ms	ms	ms	ms
math functions	$_{ m ms}$	$_{ m ms}$	$_{ m ms}$	ms	$_{ m ms}$	$_{ m ms}$
e2q, q2e	+	+	_	_	_	_
A2T, T2A	_	_	+	_	_	-
clip_wl	+	+	+	+	+	+
trim_wl	+	+	+	+	+	+
(trim_mspct)	+	+	+	+	+	+
interpolate_wl	+	+	+	+	+	+
(interpolate_mspct)	+	+	+	+	+	+
fscale	+	+	+	+	_	_
fshift	+	+	+	+	_	_
normalize	+	+	+	+	_	_
clean	+	+	+	+	_	_
tag	+	+	+	+	+	+
untag	+	+	+	+	+	+

```
## Time unit: 1s
##
##
     w.length s.e.irrad spct.idx s.q.irrad
rbindspct(list(A = sun.spct, B = shade.spct), idfactor = "site")
## Object: source_spct [1,044 x 4]
## Wavelength (nm): range 280 to 800, step -520 to 1
## Time unit: 1s
##
##
   w.length s.e.irrad site s.q.irrad
##
      (dbl) (dbl) (fctr) (dbl)
## 1 280.0000 0 A 0
## 2 280.9231 0 A 0
## 3 281.8462
## 4 282.7692
                 O A
                               0
                 0
                        A
                                0
```

In the special case when the members of the list are <code>source_spct</code> objects containing effective spectral irradiance data, and they are not based on the same BSWF, an additional factor BSWF will be automatically added, and the BSWF attribute of the resulting spectrum set to "multiple".

```
rbindspct(list(sun.spct * CIE(), sun.spct * GEN.G()))
## Error in rbindspct(list(sun.spct * CIE(), sun.spct * GEN.G())): could not
find function "CIE"
```

Special *Extract* methods for spectral objects have been implemented. These are used by default and preserve the attributes used by this package, except when the returned value is a single column from the spectral object.

```
sun.spct[1:10, ]
## Object: source_spct [10 x 3]
## Wavelength (nm): range 280 to 288.30769, step 0.9230769
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
## (dbl) (dbl) (dbl)
## 1 280.0000 0 0
                   0 0
                0
## 2 280.9231
## 3 281.8462
## 4 282.7692
                  0 0 0
## ..
      . . .
                   . . .
sun.spct[1:10, 1]
```

```
## [1] 280.0000 280.9231 281.8462 282.7692 283.6923 284.6154 285.5385
## [8] 286.4615 287.3846 288.3077

sun.spct[1:10, 1, drop = TRUE]

## [1] 280.0000 280.9231 281.8462 282.7692 283.6923 284.6154 285.5385
## [8] 286.4615 287.3846 288.3077

sun.spct[1:10, "w.length", drop = TRUE]

## [1] 280.0000 280.9231 281.8462 282.7692 283.6923 284.6154 285.5385
## [8] 286.4615 287.3846 288.3077
```

In contrast to trim_spct, subset never interpolates or inserts *hinges*. On the other hand, the subset argument accepts any logical expression and can be consequently used to do subsetting, for example, based on factors. Both subset() and trim() methods preserve attributes.

```
subset(sun.spct, s.e.irrad > 0.2)
## Object: source_spct [475 x 3]
## Wavelength (nm): range 324 to 800, step 1 to 3
## Time unit: 1s
##
    w.length s.e.irrad s.q.irrad
      (dbl) (dbl)
##
                             (dbl)
         324 0.2075508 5.621282e-07
## 1
## 2
          325 0.2168055 5.890059e-07
## 3
         326 0.2774416 7.560580e-07
## 4
        327 0.2851096 7.793375e-07
## ..
subset(sun.spct, w.length > 600)
## Object: source_spct [200 x 3]
## Wavelength (nm): range 601 to 800, step 1
## Time unit: 1s
##
##
     w.length s.e.irrad
                        s.q.irrad
##
      (dbl) (dbl)
        601 0.6295837 3.162962e-06
## 1
## 2
         602 0.6305890 3.173284e-06
## 3
          603 0.6360329 3.205995e-06
          604 0.6578140 3.321284e-06
## 4
## ..
subset(sun.spct, c(TRUE, rep(FALSE, 99)))
## Object: source_spct [6 x 3]
## Wavelength (nm): range 280 to 779, step 99 to 100
## Time unit: 1s
##
##
    w.length s.e.irrad
                        s.q.irrad
      (dbl) (dbl)
##
## 1 280 0.0000000 0.000000e+00
```

R's Extract methods \$ and [[]] can be used to extract whole columns. Replace methods \$<- and [<- have definitions for spectral objects, which allow their safe use. They work identically to those for data frames but check the validity of the spectra after the replacement.

8.2 Conversions between radiation units

The functions e2q and q2e can be used on source spectra to convert spectral energy irradiance into spectral photon irradiance and vice versa. A second optional argument sets the action with "add" and "replace" as possible values. By default these functions use normal reference semantics.

```
e2q(sun.spct, "add")
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
      w.length s.e.irrad s.q.irrad
      (dbl) (dbl) (dbl)
##
## 1 280.0000 0 0
## 2 280.9231 0 0
## 3 281.8462 0 0
## 4 282.7692 0 0
e2q(sun.spct, "replace")
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.q.irrad
##
       (dbl) (dbl)
                0
## 1 280.0000
## 2 280.9231
                       0
                0
## 3 281.8462
## 4 282.7692
```

For filter_spct objects functions T2A and A2T allow conversion between spectral transmittance and spectral absorbance and vice versa.

8.3 Normalizing a spectrum

Function normalize permits normalizing a spectrum to a value of one at an arbitrary wavelength (nm) or to the wavelength of either the maximum or the minimum spectral value. It supports the different spectral classes, we use a source_spct object as an example.

```
normalize(sun.spct)
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
## Spectral data normalized to 1 at 451 \text{ nm}
##
      w.length s.e.irrad
##
       (dbl) (dbl)
## 1 280.0000
                      0
## 2 280.9231
                      0
## 3 281.8462
## 4 282.7692
                      0
```

Which is equivalent to supplying "max" as argument to norm, it is also possible to give a range within which the maximum should be searched.

```
normalize(sun.spct, range = PAR(), norm = "max")
## Error in normalize_spct(spct = q2e(x, action = "replace"), range = range, :
could not find function "PAR"
```

It is also possible to normalize to an arbitrary wavelength within the range of the data, even if it is not one of the wavelength values present in the spectral object, as interpolation is used when needed.

```
normalize(sun.spct, norm = 600.3)
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
## Spectral data normalized to 1 at 600.3 nm
##
##
     w.length s.e.irrad
##
      (dbl) (dbl)
## 1 280.0000
                  0
## 2 280.9231
                     0
## 3 281.8462
                      0
## 4 282.7692
                     0
## ..
```

8.4 Rescaling a spectrum

Function fscale() rescales a spectrum by dividing each spectral data value by a value calculated with a function (f) selected by a character string ("total" or "mean"), or an actual R function which can accept the spectrum object supplied as its first argument.

```
fscale(sun.spct)
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
## Rescaled to 'mean' = 1
##
     w.length s.e.irrad
##
      (dbl) (dbl)
## 1 280.0000
## 2 280.9231
                    0
## 3 281.8462
## 4 282.7692
                     0
## .. ...
fscale(sun.spct, f = "total")
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1 \,
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
## Rescaled to 'total' = 1
##
##
    w.length s.e.irrad
##
       (dbl) (dbl)
## 1 280.0000
                  0
## 2 280.9231
                    0
## 3 281.8462
                     0
## 4 282.7692
                     0
## ..
fscale(sun.spct, range = PAR(), f = irrad)
## Error in fscale_spct(spct = q2e(x, action = "replace"), range = range, :
could not find function "PAR"
```

In the third example, the spectral data is rescaled so that the corresponding photosynthetically-active irradiance is equal to one.

8.5 Shifting the zero of the spectral data scale

Function fshift() shifts the zero of the scale of a spectrum by subtracting from each spectral data value a value calculated with a function (f) selected by a character string ("mean", "min" or "max"), or an actual R function which can

accept the spectrum object supplied as its first argument. The range argument selects a region of the spectrum to be used as *reference* in the calculation of the summary.

```
fshift(sun.spct, range = UVB(), f = "mean")
## Error in fshift_spct(spct = q2e(x, action = "replace"), range = range, :
could not find function "UVB"
fshift(sun.spct, range = c(280,290), f = "min")
## Object: source_spct [522 x 2]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
    w.length s.e.irrad
##
       (dbl) (dbl)
                  0
## 1 280.0000
## 2 280.9231
                      0
## 3 281.8462
                     0
## 4 282.7692
```

In the first example, the spectral data shifted so that the mean spectral irradiance becomes zero for the UV-B region. In the second example the minimum value in the range of wavelengths between 280 nm and 290 nm is used as zero reference for the scale.

8.6 Replacing off-range spectral data values

Method clean() should be used with care as off-range values stem almost always from calibration errors or measuring noise. This function allows one to replace such values, but in many cases a zero shift or rescaling could be the option to be preferred. Even when the off-range values are the result of random noise, replacing them with the boundary values can cause bias, by censoring the data. Here we create *artificial* off-range values by subtracting a constant from each spectrum.

```
clean(sun.spct - 0.01, range = c(280.5, 282))

## Warning in range_check(x, strict.range = strict.range): Negative spectral
energy irradiance values; minimum s.e.irrad = -0.01

## Object: source_spct [522 x 2]

## Wavelength (nm): range 280 to 800, step 0.9230769 to 1

## Measured on: 2010-06-22 09:51:00 UTC

## Measured at: 60.20942 N, 24.96424 E

## Time unit: 1s

##

## w.length s.e.irrad

## (db1) (db1)
```

```
clean(polyester.spct - 0.053)
## Object: filter_spct [611 x 2]
## Wavelength (nm): range 190 to 800, step 1
##
##
     w.length Tfr
##
        (int) (dbl)
## 1
          190
## 2
          191
                  0
## 3
          192
                  0
## 4
         193
## ..
```

8.7 Wavelength interpolation

Converting spectra available at a given set of wavelengths values to a different one, is frequently needed when operating with several spectra of different origin. One can increase the *apparent* resolution by interpolation, and reduce it by local averaging or smoothing and resampling. The same function works on all spct objects, interpolating every column except w.length and replacing in this last column the old wavelength values with the new ones supplied as argument. The optional argument fill.value control what value is assigned to wavelengths in the new data that are outside the range of the old wavelengths.

```
interpolate_wl(sun.spct, seq(400, 500, by = 0.1))
## Object: source_spct [1,001 x 3]
## Wavelength (nm): range 400 to 500, step 0.1
## Time unit: 1s
##
     w.length s.e.irrad s.q.irrad
##
##
      (dbl) (dbl)
                        (dbl)
## 1
        400.0 0.6081049 2.033314e-06
## 2
        400.1 0.6099118 2.039879e-06
       400.2 0.6117187 2.046445e-06
## 3
## 4
       400.3 0.6135257 2.053010e-06
## ..
```

8.8 Trimming and clipping

8.8.1 Method clip_wl()

Sometimes it is desirable to change the range of wavelengths included in a spectrum. If we are interested in a given part of the spectrum, there is no need

to do calculations or plotting the whole spectrum. To select part a spectrum based on a range of wavelengths we may use the clip_wl method.

The range of wavelengths expressed in nanometres can be given as numeric vector of length two.

```
clip_wl(sun.spct, range = c(400, 402))
## Object: source_spct [3 x 3]
## Wavelength (nm): range 400 to 402, step 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
    w.length s.e.irrad s.q.irrad
    (dbl) (dbl) (dbl)
## 1
         400 0.6081049 2.033314e-06
## 2
         401 0.6261742 2.098967e-06
## 3
         402 0.6497388 2.183388e-06
clip_wl(sun.spct, range = c(400, NA))
## Object: source_spct [401 x 3]
## Wavelength (nm): range 400 to 800, step 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
       v.length s.e.irrad s.q.irrad (dbl) (dbl) (dbl)
     w.length s.e.irrad
##
         400 0.6081049 2.033314e-06
## 2
         401 0.6261742 2.098967e-06
## 3
          402 0.6497388 2.183388e-06
## 4
          403 0.6207287 2.091091e-06
## ..
```

As for trim_w1() the range can be also supplied as a waveband object, or any other object for which range() returns a numeric range. Even a different spectrum object is acceptable.

```
clip_wl(sun.spct, range = UVA)
## Object: source_spct [86 x 3]
## Wavelength (nm): range 315 to 400, step 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
##
      (dbl) (dbl)
        315 0.1127901 2.969940e-07
## 1
## 2 316 0.1020587 2.695897e-07
        317 0.1487690 3.942191e-07
## 3
## 4
         318 0.1413919 3.758526e-07
                . . .
```

The result can be a spectrum of length zero.

```
clip_wl(sun.spct, range = c(100, 200))

## Object: source_spct [0 x 3]

## Measured on: 2010-06-22 09:51:00 UTC

## Measured at: 60.20942 N, 24.96424 E

## Time unit: 1s

##

## Variables not shown: w.length (dbl), s.e.irrad (dbl), s.q.irrad (dbl)
```

8.8.2 Method trim_wl()

Sometimes, we need more flexibility. We may want to replace the observed values outside a certain range or expand the range of wavelengths, filling the expansion of all other variables with a certain value (i.e. a number, or NA.). In contrast to *clipping* (or functionally equivalent, indexing, or subsetting), *trimming* ensures that there will be spectral data returned at the boundaries of the trimmed region. These values are obtained by interpolation when they are not already present in the data.

More flexibility is available in method trim_wl(), to which we can supply arguments range, use.hinges, and fill. By default interpolation is used at the boundaries of the range.

```
trim_wl(sun.spct, c(282.5, NA))
## Object: source_spct [520 x 3]
## Wavelength (nm): range 282.5 to 800, step 0.2692308 to 1
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
##
       (dbl) (dbl) (dbl)
                 0
                           0
## 1 282.5000
                    0
## 2 282.7692
                              0
## 3 283.6923
                     0
                               0
## 4 284.6154
                     0
                               0
## ..
clip_wl(sun.spct, c(282.5, NA))
## Object: source_spct [519 x 3]
## Wavelength (nm): range 282.76923 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
       (dbl) (dbl) (dbl)
##
## 1 282.7692 0
## 2 283.6923 0
## 3 284.6154 0
## 4 285.5385 0
                            0
                               0
                               0
                               0
## .. ...
```

As for clip_wl() the range can be also supplied as a waveband object, or any other object for which range() returns a numeric range. Even a different spectrum object is acceptable.

```
trim_wl(sun.spct, PAR())
## Error in trim_wl.generic_spct(sun.spct, PAR()): could not find function "PAR"
```

The default for fill is NULL which results in deletion values outside the trimmed region. However, it is possible to supply a different argument, to be used to replace the off-range data values.

Furthermore, when fill is not NULL, expansion is possible.

```
trim_wl(sun.spct, c(275, NA), fill = 0)
## Object: source_spct [529 x 3]
## Wavelength (nm): range 275 to 800, step 1.023182e-12 to 1
## Time unit: 1s
##
##
   w.length s.e.irrad s.q.irrad
##
      (dbl) (dbl) (dbl)
               0
## 1 275.0000
                   0
## 2 275.8333
                            0
## 3 276.6667
                  0
                           0
## 4 277.5000
                            0
                   0
## .. ...
```

By default interpolation at the boundaries is used, but setting use.hinges to FALSE results in clipping, a behaviour similar to that of clip_wl only if fill == NULL.

```
trim_wl(sun.spct, c(281.5, NA), fill = NA)

## Object: source_spct [524 x 3]
## Wavelength (nm): range 280 to 800, step 1.023182e-12 to 1
## Time unit: 1s
##
## w.length s.e.irrad s.q.irrad
## (dbl) (dbl) (dbl)
```

```
## 1 280.0000 NA
                              NA
## 2 280.9231
                              NA
                    NΑ
## 3 281.5000
                    NA
                              NA
## 4 281.5000
                   0
                              0
        . . .
                   . . .
                             . . .
trim_wl(sun.spct, c(281.5, NA), fill = NA, use.hinges = FALSE)
## Object: source_spct [522 x 3]
## Wavelength (nm): range 280 to 800, step 0.9230769 to 1
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad s.q.irrad
##
       (dbl) (dbl) (dbl)
## 1 280,0000
                           NA
                  NA
## 2 280.9231
                    NA
                             NA
## 3 281.8462
                    0
                              0
## 4 282.7692
                    0
                               0
```

When use.hinges == TRUE and expanssion or replacement is done, two observations are inserted at each boundary, differing in wavelength by 1×10^{-12} nm to prevent rounding errors in later calculations.

8.8.3 Functions trim_spct and trim_spct

Functions trim_spct and trim_spct are not generic, and add even more flexibility, but trim_wl should be preferred in user scripts.

8.9 Convolving weights

It is very instructive to look at weighted spectral data to understand how effective irradiances are calculated. Plotting effective spectral irradiance data can be very instructive when analyzing the interaction of photoreceptors and ambient radiation. It can also illustrate what a large effect that small measuring errors can have on the estimated effective irradiances or exposures when SWFs have a steep slope.

8.9.1 Individual spectra

The multiplication operator is defined for operations between a source_spct and a waveband, so this is the easiest way of doing the calculations.

```
sun.spct * CIE()
## Error in eval(expr, envir, enclos): could not find function "CIE"
```

8.9.2 Vectors

It is also possible to use vectors.

8.10 Tagging with bands and colours

We call tagging, to the process of adding reference information to spectral data. For example we can add a factor indicating regions or bands in the spectrum. We can add also information on the colour, as seen by humans, for each observed value, or for individual regions or bands of the spectrum. In most cases this additional information is used for annotations when plotting the spectral data.

8.10.1 Individual spectra

The function tag can be used to tag different parts of a spectrum according to wavebands.

```
tag(sun.spct, PAR(), byref = FALSE)
## Error in tag.generic_spct(sun.spct, PAR(), byref = FALSE): could not find
function "PAR"

tag(sun.spct, UV_bands(), byref = FALSE)
## Error in tag.generic_spct(sun.spct, UV_bands(), byref = FALSE): could not find
function "UV_bands"
```

The added factor and colour data can be used for further processing or for plotting. Information about the tagging and wavebands is stored in an attribute tag.attr in every tagged spectrum, this yields a more compact output and keeps a 'trace' of the tagging.

```
tg.sun.spct <- tag(sun.spct, PAR(), byref = FALSE)

## Error in tag.generic_spct(sun.spct, PAR(), byref = FALSE): could not find
function "PAR"

attr(tg.sun.spct, "spct.tags")

## Error in eval(expr, envir, enclos): object 'tg.sun.spct' not found</pre>
```

Additional functions are available which return a tagged spectrum and take as input a list of wavebands, but no spectral data. They 'build' a spectrum from the data in the wavebands, and are useful for plotting the boundaries of wavebands.

```
wb2tagged_spct(UV_bands())
## Error in is.waveband(w.band): could not find function "UV_bands"
wb2rect_spct(UV_bands())
## Error in is(w.band, "waveband"): could not find function "UV_bands"
```

Function wb2tagged_spct returns a tagged spectrum, with two rows for each waveband, corresponding to the low and high wavelength boundaries, while function wb2rect_spct returns a spectrum with only one row per waveband, with w.length set to its midpoint but with additional columns xmin and xmax corresponding to the low and high wavelength boundaries of the wavebands.

Function is_tagged can be used to query if an spectrum is tagged or not, and function untag removes the tags.

```
## Error in eval(expr, envir, enclos): object 'tg.sun.spct' not found
is_tagged(tg.sun.spct)
## Error in is.any_spct(x): object 'tg.sun.spct' not found
untag(tg.sun.spct)
## Error in untag(tg.sun.spct): object 'tg.sun.spct' not found
is_tagged(tg.sun.spct)
## Error in is.any_spct(x): object 'tg.sun.spct' not found
```

In the chuck above, we can see how this works, using in this case the default byref = TRUE which adds the tags in place, or "by reference", to the spct object supplied as argument.

9 Summaries

Summaries can be calculated both from individual spectral objects (Table 10) and from collections of spectral objects (Table 11). They return a *simpler* object than the spectral data in their arguments. For example a vector of numeric values, possibly of length one, in the case of individual spectra, or a data frame containing one row of summary data for each spectrum the collection of multiple spectra supplied as argument.

9.1 Summary

Specialized definitions of summary and the corresponding print methods are available for spectral objects. In the case of source_spct objects the time.unit attribute makes it possible to print the summary using the correct units.

Table 10: Summary methods for spectra. Key: + available, - not available.

methods	source	response	filter	reflector	object	chroma
irrad	+	-	_	-	_	-
$e_{-}irrad$	+	_	_	_	_	_
$q_{-}irrad$	+	_	_	_	_	_
fluence	+	_	_	_	_	_
e_fluence	+	_	_	_	_	_
q_{-} fluence	+	_	_	_	_	_
ratio	+	_	_	_	_	_
e_{-} ratio	+	_	_	_	_	_
$q_{\mathtt{ratio}}$	+	_	_	_	_	_
qe_ratio	+	_	_	_	_	_
eq_ratio	+	_	_	_	_	_
response	_	+	_	_	_	-
e_response	_	+	_	_	_	_
q_{-} response	_	+	_	_	_	-
transmittance	_	_	+	_	+	_
absorptance	_	_	+	_	+	_
absorbance	_	_	+	_	+	_
reflectance	_	_	_	+	+	_
range	+	+	+	+	+	+
min	+	+	+	+	+	+
max	+	+	+	+	+	+
stepsize	+	+	+	+	+	+
spread	+	+	+	+	+	+
${\tt midpoint}$	+	+	+	+	+	+
labels	+	+	+	+	+	+
summary	+	+	+	+	+	+
peaks	+	+	+	+	(+)	(+)
valleys	+	+	+	+	(+)	(+)
$integrate_spct$	+	+	+	+	+	+
$average_spct$	+	+	+	+	+	+
color	+	_	_	_	-	_

Table 11: Summary methods for collections of spectra. Key: + available, - not available, ms use msmsply() to apply function to collection members, d use msdply(), l use mslply to apply function to collection members, a use msaply to apply function to collection members.

methods	source	response	filter	reflector	object	chroma
f_mspct	+	+	+	+	+	+
irrad	+	-	-	-	-	-
e_{-} irrad	+	_	_	_	_	_
$q_{ extsf{-}}irrad$	+	_	_	_	_	_
fluence	+	_	-	_	-	-
e_{-} fluence	+	_	_	_	_	_
q_{-} fluence	+	_	_	_	_	_
ratio	+	_	-	_	-	-
e_ratio	+	_	_	_	_	_
q _ratio	+	_	-	_	-	-
qe_ratio	+	_	_	_	_	_
eq_ratio	+	-	-	_	-	-
response	_	+	-	_	_	_
$e_response$	_	+	-	_	_	_
$q_response$	_	+	-	_	-	-
transmittance	_	-	+	_	+	-
absorptance	_	-	+	_	+	_
absorbance	_	_	+	_	+	_
reflectance	_	-	-	+	+	-
range	+	+	+	+	+	+
min	+	+	+	+	+	+
max	+	+	+	+	+	+
stepsize	+	+	+	+	+	+
spread	+	+	+	+	+	+
${\tt midpoint}$	+	+	+	+	+	+
labels	1	1	1	1	1	1
summary	l	1	1	1	1	1
peaks	+	+	+	+	(+)	(+)
valleys	+	+	+	+	(+)	(+)
$integrate_spct$	a, d, l	a, d, l	a, d, l	a, d, l	a, d, l	a, d, l
$average_spct$	a, d, l	a, d, l	a, d, l	a, d, l	a, d, l	a, d, l
color	+	-	_	_	_	_

```
## Summary (sun.spct)

## Summary of object: source_spct [522 x 3]

## Wavelength (nm): range 280 to 800, step 0.9230769 to 1

## Measured on: 2010-06-22 09:51:00 UTC

## Measured at: 60.20942 N, 24.96424 E

## Time unit: 1s

##

## w.length s.e.irrad s.q.irrad

## Min. :280.0 Min. :0.0000 Min. :0.000e+00

## 1st Qu.:409.2 1st Qu.:0.4115 1st Qu.:1.980e-06

## Median :539.5 Median :0.5799 Median :2.929e-06

## Mean :539.5 Mean :0.5160 Mean :2.407e-06

## 3rd Qu.:669.8 3rd Qu.:0.6664 3rd Qu.:3.154e-06

## Max. :800.0 Max. :0.8205 Max. :3.375e-06
```

9.2 Wavelength

9.2.1 Individual spectra

The 'usual' and a couple of new summary functions are available for spectra, but redefined to return wavelength based summaries in nanometres (nm).

```
range(sun.spct)
## [1] 280 800
min(sun.spct)
## [1] 280
max(sun.spct)
## [1] 800
midpoint(sun.spct)
## [1] 540
spread(sun.spct)
## [1] 520
stepsize(sun.spct)
## [1] 0.9230769 1.0000000
```

9.2.2 Collections of spectra

Most frequently used summary methods are implemented for collections of spectra. See Table 11 where methods that need to be applied with functions msaply, msdply or mslply to members in a collection and obtain the results in an array (vector, or matrix), a data frame or a list object are indicated. In many cases depending of the class desired for the result, one can chose a suitable 'apply' function, and sometimes it is best to use such a function, even when the corresponding method is implemented for collections of spectra.

Collections of spectra can be useful not only for time-series of spectra or spectral images, but also when dealing with a small group of related spectra. In the example below we show how to use a collection of spectra for calculating summaries. The spectra in a collection do **not** need to have been measured at the same wavelength values, or have the same number of rows or even of columns. Consequently, in many cases applying the wavelength summary functions described above to collections of spectra can be useful. The value returned is a data frame, with a number of data columns equal to the length of the returned value by the corresponding method for individual spectra.

```
filters.mspct <- filter_mspct(list(none = clear.spct,</pre>
                                 pet = polyester.spct,
                                 yellow = yellow.gel.spct))
range(filters.mspct)
## Source: local data frame [3 x 3]
##
##
    spct.idx min.wl max.wl
##
     (fctr) (dbl) (dbl)
       none
## 1
              100
                     5000
       pet 190
## 2
                     800
## 3 yellow
              190
                       800
```

9.3 Peaks and valleys

9.3.1 Individual spectra

Functions peaks and valleys take spectra as first argument and return a subset of the spectral object data corresponding to local maxima and local minima of the measured variable. span defines the width of the 'window' used as a number of observations.

```
peaks(sun.spct, span = 51)

## Object: source_spct [3 x 2]
## Wavelength (nm): range 451 to 747, step 44 to 252
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
```

```
##
##
    w.length s.e.irrad
##
      (dbl)
                 (dbl)
## 1
        451 0.8204633
## 2
         495 0.7899872
## 3
        747 0.5025733
valleys(sun.spct, span = 51)
## Object: source_spct [9 x 2]
## Wavelength (nm): range 358 to 761, step 30 to 72
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.e.irrad
##
       (dbl) (dbl)
## 1
          358 0.2544907
## 2
          393 0.2422023
## 3
          431 0.4136900
## 4
         487 0.6511654
## ..
```

In the case of source_spct and response_spct methods unit.out can be used to force peaks to be searched using either energy or photon based spectral irradiance. The default is energy, or the option "photobiology.radiation.unit" if set.

```
peaks(sun.spct, span = 51, unit.out = "photon")
## Object: source_spct [7 x 2]
## Wavelength (nm): range 451 to 754, step 36 to 90
## Measured on: 2010-06-22 09:51:00 UTC
## Measured at: 60.20942 N, 24.96424 E
## Time unit: 1s
##
##
     w.length s.q.irrad
##
       (dbl)
                     (dbl)
## 1
          451 3.093155e-06
## 2
          495 3.268822e-06
## 3
         531 3.374912e-06
## 4
         621 3.355564e-06
## ..
```

It is possible to approximately set the width of the windows in nanometres by using function step_size. However, here we simply use an odd number of wavelengths 'steps'.

```
peaks(sun.spct, span = 21)

## Object: source_spct [18 x 2]

## Wavelength (nm): range 354 to 774, step 11 to 51

## Measured on: 2010-06-22 09:51:00 UTC

## Measured at: 60.20942 N, 24.96424 E

## Time unit: 1s
```

Low level functions find_peaks, get_peaks and get_valleys take numeric vectors as arguments.

9.3.2 Collections of spectra

We can use msmsply() to extract the peaks of a collection of spectra.

```
msmsply(filters.mspct, peaks, span = 11)
## Object: filter_mspct [3 x 1]
## --- Member: none ---
## Object: filter_spct [0 x 2]
## Variables not shown: w.length (dbl), Tfr (dbl)
## --- Member: pet ---
## Object: filter_spct [8 x 2]
## Wavelength (nm): range 453 to 648, step 6 to 76
##
##
    w.length Tfr
       (int) (dbl)
##
## 1
         453 0.926
## 2
          503 0.926
         579 0.921
## 3
        609 0.919
## ..
## --- Member: yellow ---
## Object: filter_spct [5 x 2]
## Wavelength (nm): range 642 to 755, step 8 to 64
##
##
     w.length
                 Tfr
##
       (int) (dbl)
## 1
          642 0.8980
## 2
          706 0.9005
## 3
          714 0.9005
## 4
          744 0.9015
## ..
## --- END ---
```

Two of the filters in the collection do not have peaks, and a spectrum object of length zero is returned for them.

9.4 Irradiance

9.4.1 Individual spectra

The code using spct objects is simple, to integrate the whole spectrum we can use

```
irrad(sun.spct)

## Total

## 269.1249

## attr(,"time.unit")

## [1] "second"

## attr(,"radiation.unit")

## [1] "energy irradiance total"
```

and, to integrate a range of wavelengths, in the example, photosynthetically active radiation, we use the predefined waveband constructor PAR().

```
irrad(sun.spct, PAR())
## Error in irrad.source_spct(sun.spct, PAR()): could not find function "PAR"
```

The default for irrad, when no argument unit.out is supplied, is to return the irradiance value in energy irradiance units, unless the R option photobiology.radiation.unit is set.

Functions e_irrad and q_irrad save some typing, and always return the same type of spectral irradiance quantity, independently of global option photobiology.radiation.unit.

```
e_irrad(sun.spct, PAR()) # W m-2

## Error in irrad_spct(spct, w.band = w.band, unit.out = "energy", quantity =
quantity, : could not find function "PAR"

q_irrad(sun.spct, PAR()) * 1e6 # umol s-1 m-2

## Error in irrad_spct(spct, w.band = w.band, unit.out = "photon", quantity =
quantity, : could not find function "PAR"
```

It is also possible to supply a time unit to use as basis of expression for the returned value, but be aware that conversion into a loger time unit is only valid for sources like lamps, which have an output the remains constant in time.

```
irrad(sun.spct, PAR(), time.unit = "hour")
## Error in irrad.source_spct(sun.spct, PAR(), time.unit = "hour"): could not
find function "PAR"

irrad(sun.spct, PAR(), time.unit = duration(8, "hours"))
## Error in irrad.source_spct(sun.spct, PAR(), time.unit = duration(8, "hours")):
could not find function "PAR"
```

Using a shorter time unit than the original, yields an average value reexpressed on a new time unit base.

```
irrad(sun.daily.spct, PAR(), time.unit = "second")
## Error in irrad.source_spct(sun.daily.spct, PAR(), time.unit = "second"):
could not find function "PAR"
```

Lists of wavebands are also accepted as argument.

```
my_wavebands <- list(Red(), Blue(), Green())

## Error in eval(expr, envir, enclos): could not find function "Red"

e_irrad(sun.spct, my_wavebands) # W m-2

## Error in irrad_spct(spct, w.band = w.band, unit.out = "energy", quantity = quantity, : object 'my_wavebands' not found</pre>
```

These functions have an additional argument quantity, with default "total", which can take values controlling the output. The value "total" yields **irradiance** in W m $^{-2}$, integrated over wavelengths for each waveband, while "average" yields the mean **spectral irradiance** within each waveband in W m $^{-2}$ nm $^{-1}$. The value "contribution" is relative to the irradiance for the whole spectrum, expressed as a fraction of one, while the value "relative" is relative to the sum of the irradiances for the different wavbands given as argument, also expressed as a fraction of one.

```
irrad(sun.spct, UV_bands(), quantity = "total")

## Error in irrad.source_spct(sun.spct, UV_bands(), quantity = "total"): could
not find function "UV_bands"

irrad(sun.spct, UV_bands(), quantity = "contribution")

## Error in irrad.source_spct(sun.spct, UV_bands(), quantity = "contribution"):
could not find function "UV_bands"

irrad(sun.spct, UV_bands(), quantity = "relative")

## Error in irrad.source_spct(sun.spct, UV_bands(), quantity = "relative"):
could not find function "UV_bands"

irrad(sun.spct, UV_bands(), quantity = "average")

## Error in irrad.source_spct(sun.spct, UV_bands(), quantity = "average"): could
not find function "UV_bands"
```

9.4.2 Collections of spectra

Collections of spectra can be useful not only for time-series of spectra or spectral images, but also when dealing with a small group of related spectra. In the example below we show how to use a collection of spectra for estimating irradiances under different filters set up in sunlight.

We reuse collection of filter spectra filters.mspct from section 9.2.2 on page 58.

```
names(filters.mspct)
## [1] "none" "pet" "yellow"
```

We then convolve each filter's spectral transmittance by the spectral irradiance of the light source

```
filtered_sun <- convolve_each(filters.mspct, sun.spct)
irrad(filtered_sun, list(UVA, PAR))

## Source: local data frame [3 x 3]

##

## spct.idx irrad_UVA irrad_PAR

## (fctr) (dbl) (dbl)

## 1 none 27.98420611 196.6343

## 2 pet 22.98282851 181.0213

## 3 yellow 0.03726539 106.9680</pre>
```

The code above can also be written as a single statement

```
irrad(convolve_each(filters.mspct, sun.spct), list(UVA, PAR))

## Source: local data frame [3 x 3]

##

## spct.idx irrad_UVA irrad_PAR

## (fctr) (dbl) (dbl)

## 1 none 27.98420611 196.6343

## 2 pet 22.98282851 181.0213

## 3 yellow 0.03726539 106.9680
```

It is also possible to use an 'apply' function. Syntax parallels that of base R's and package plyr's. See sections 4.5 and 4.6 for more details.

One thing to remember, is that operators in R are just normal functions with special names and call syntax. They can also be called with the usual function call syntax by enclosing their *name* in backquotes. We use this to pass as argument the multiplication operator '*' in a call to msmsply which returns, in this case, a source_multi_spct object. After this we just call the irrad method on the *collection of spectra* and obtain the result as a data frame with one row per spectrum and one column by waveband.

```
filtered_sun <- msmsply(filters.mspct, `*`, sun.spct)
irrad(filtered_sun, list(UVA, PAR))

## Source: local data frame [3 x 3]

##

## spct.idx irrad_UVA irrad_PAR

## (fctr) (dbl) (dbl)

## 1 none 27.98420611 196.6343

## 2 pet 22.98282851 181.0213

## 3 yellow 0.03726539 106.9680</pre>
```

9.4.3 Numeric vectors

The code using numeric vectors is more complicated, but adds some additional flexibility for tweaking performance. Under normal circumstances it is easier to use the functions described above.

Function irradiance takes an array of wavelengths (sorted in strictly increasing order), and the corresponding values of spectral irradiance. By default the input is assumed to be in energy units, but parameter unit.in can be used to change this default. The type of unit used for the returned quantity is set by unit.out with no default. The behaviour with respect to wavebands is as described above for spectral objects. The functions photon_irradiance() and energy_irradiance(), just call irradiance() with the unit.out set to "photon" or "energy" respectively.

The functions taking numerical vectors as arguments can be used with data stored as vectors, or using with with data frames, data tables, lists, and spectra objects.

```
with(sun.spct, photon_irradiance(w.length, s.e.irrad, PAR))
## PAR
## 0.0008941352
```

The recommended practice is to use with, as above.

9.5 Fluence

9.5.1 Individual spectra

The calculation of fluence values (time-integrated irradiance) is identical to that for irradiance, except that a exposure.time argument needs to be supplied. The exposure time must be a lubridate::duration, but any argument accepted by as.duration can also be used. Functions fluence, e_fluence and q_fluence correspond to irrad, e_irrad and q_irrad,

```
fluence(sun.spct, exposure.time = duration(1, "hours"))
##
     Total
## 968849.6
## attr(,"radiation.unit")
## [1] "energy fluence (J m-2)"
## attr(,"exposure.duration")
## [1] "3600s (~1 hours)"
fluence(sun.spct, exposure.time = 3600) # seconds
## converting 'time.unit' 3600 into a lubridate::duration
##
     Total
## 968849.6
## attr(,"radiation.unit")
## [1] "energy fluence (J m-2)"
## attr(,"exposure.duration")
## [1] 3600
```

```
fluence(sun.spct, exposure.time = hms("01:00:00"))

## converting 'time.unit' 1H OM OS into a lubridate::duration
## estimate only: convert periods to intervals for accuracy

## Total
## 968849.6

## attr(,"radiation.unit")

## [1] "energy fluence (J m-2)"

## attr(,"exposure.duration")

## [1] "1H OM OS"
```

and, to obtain the photon fluence for a range of wavelengths, in the example, photosynthetically active radiation, we use the PAR waveband object earlier defined, for 25 minutes of exposure.

```
e_fluence(sun.spct, PAR, exposure.time = hms("00:25:00"))

## converting 'time.unit' 25M OS into a lubridate::duration
## estimate only: convert periods to intervals for accuracy

## PAR
## 294951.4
## attr(,"radiation.unit")
## [1] "energy fluence (J m-2)"
## attr(,"exposure.duration")
## [1] "25M OS"
```

9.6 Photon and energy ratios

9.6.1 Individual spectra

The functions described here, in there simplest use, calculate a ratio between two wavebands. The function q_ratio returning photon ratios. However both waveband parameters can take lists of wavebands as arguments, with normal recycling rules in effect. The corresponding function e_ratio returns energy ratios.

```
q_ratio(sun.spct, UVB, PAR)
## UVB: PAR(q:q)
    0.001873724
## attr(,"radiation.unit")
## [1] "q:q ratio"
q_ratio(sun.spct,
       list(UVC, UVB, UVA,
        UV))
##
        UVB: Total(q:q)
                              UVA: Total(q:q) UV.tr.lo: Total(q:q)
            0.001334593
                                  0.067567343
                                                         0.068901936
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

Function qe_ratio, has only one waveband parameter, and returns the 'photon' to 'energy' ratio, while its complement eq_ratio returns the 'energy' to 'photon' ratio.

```
qe_ratio(sun.spct, list(UVB, PAR))

## q:e( UVB) q:e( PAR)

## 2.599434e-06 4.547199e-06

## attr(,"radiation.unit")

## [1] "q:e ratio"
```

9.6.2 Collections of spectra

```
q_ratio(filtered_sun, list(UVB, UVA, PAR))

## Source: local data frame [3 x 4]

##

## spct.idx q_ratio_UVB:Total(q:q) q_ratio_UVA:Total(q:q)

## (fctr) (dbl) (dbl)

## 1 none 1.334593e-03 0.0675673430

## 2 pet 3.700698e-05 0.0614239749

## 3 yellow 2.540715e-06 0.0001339225

## Variables not shown: q_ratio_PAR:Total(q:q) (dbl)
```

9.6.3 Vectors

The function waveband_ratio() takes basically the same parameters as irradiance, but two waveband definitions instead of one, and two unit.out definitions instead of one. This is the base function used in all the vector based 'ratio' functions in the photobiology package.

Similar functions photon_ratio(), energy_ratio(), and photons_energy_ratio return the other ratios described above. In contrast to the functions described in the previous section, these functions only accept individual waveband definitions (not lists of them).

To calculate the photon ratio between UVB and PAR photon irradiance in these to regions we use.

9.7 Normalized difference indexes

9.8 Individual spectra

These indexes are frequently used to summarize reflectance data, for example in remote rensing the NDVI (normalized difference vegetation index). Here we give an *unusual* example to demonstrate that function normalized_diff_ind() can be used to calculate, or define any similar index.

9.9 Transmittance, reflectance, absorptance and absorbance

9.9.1 Individual spectra

The functions transmittance, absorptance and absorbance take filter_spct as argument, while function reflectance takes reflector_spct objects as argument. Functions transmittance, reflectance and absorptance are also implemented for object_spct. These functions return as default an average value for these quantities assuming a light source with a flat spectral energy output, but this can be changed as described above for irrad().

It is more likely that we would like to calculate these values with reference to light of a certain spectral quality. This needs to be calculated by hand, which is not difficult.

```
irrad(sun.spct * polyester.spct, list(UVB, UVA, PAR, wb.trim = TRUE)) /
    irrad(sun.spct, list(UVB, UVA, PAR, wb.trim = TRUE))

## UVB UVA PAR
## 0.02506541 0.82127856 0.92059898
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

9.9.2 Collections of spectra

Here we construct a collection of filter spectra, and then we calculate the transmittance of these filters for two wavebands, obtaining the results as a data frame, with one row per filter, and one column per waveband. We reuse once more filters.mspct from section 9.2.2 on page 58.

```
transmittance(filters.mspct, list(UVA, PAR))

## Source: local data frame [3 x 3]

##

## spct.idx transmittance_UVA transmittance_PAR

## (fctr) (dbl) (dbl)

## 1 none 1.000000000 1.00000000

## 2 pet 0.782682353 0.9202450

## 3 yellow 0.001601353 0.5655132
```

9.10 Integrated response

9.10.1 Individual spectra

The functions response, e_response and q_response take response_spct objects as arguments, and return the integrated value for each waveband (integrated over wavelength) assuming a light source with a flat spectral energy or photon output respectively. If no waveband is supplied as argument, the whole spectrum is integrated.

```
response(photodiode.spct)

## Total
## 25.37446
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy response total"
```

When a waveband, or list of wavebands, is supplied the response is calculated for the wavebands.

```
e_response(photodiode.spct, list(UVB, UVA))

## UVB UVA

## 0.7002548 5.9818181

## attr(,"time.unit")

## [1] "second"

## attr(,"radiation.unit")

## [1] "energy response total"
```

This function has an additional argument quantity, with default "total", as described for irrad().

9.10.2 Collections of spectra

9.11 Integration over wavelengths

When we need to integrate some *non-standard* numeric variable stored in a spectral object we can use functions integrate_spct or average_spct.

9.11.1 Calculation from individual spectra

We can integrate the values of arbitrary numeric columns other than w.length in an spectral object. All spectral classes are derived from generic_spct, so the examples in this section apply to objects of any of the derived spectral classes as well.

```
integrate_spct(sun.spct)
## e.irrad q.irrad
## 2.691249e+02 1.255336e-03
```

The function <code>average_spct</code> integrates every column holding numeric values from a spectrum object, except for <code>w.length</code>, and divides the result by the <code>spread</code> or width of the wavelength range integrated, returning a value expressed in the same units as the spectral data.

```
average_spct(sun.spct)
## e.irrad q.irrad
## 5.175479e-01 2.414107e-06
```

10 Astronomy

10.1 Position of the sun

In photobiology research we sometimes need to calculate the position on the sun at arbitrary locations and positions. The function sun_angles returns the azimuth in degrees eastwards, altitude in degrees above the horizon, solar disk diameter in degrees and sun to earth distance in astronomical units. The time

should be a POSIXct vector, possibly of length one, and it is easiest to use package lubridate for working with time and dates.

```
sun_angles(now(), lat = 34, lon = 0)
## $time
## [1] "2015-12-13 19:14:44 EET"
##
## $azimuth
## [1] 245.4433
##
## $elevation
## [1] -5.137191
##
## $diameter
## [1] 0.541622
## $distance
## [1] 0.9844504
sun_angles(ymd_hms("2014-01-01 0:0:0", tz = "UTC"))
## $time
## [1] "2014-01-01 UTC"
## $azimuth
## [1] 181.9507
##
## $elevation
## [1] -66.96255
##
## $diameter
## [1] 0.5422513
##
## $distance
## [1] 0.9833078
```

When spectra contain suitable metadata, the position of the sun for the spectral irradiance data measurement can be easily obtained.

```
sun_angles(getWhenMeasured(sun.spct), geocode = getWhereMeasured(sun.spct))

## $time
## [1] "2010-06-22 09:51:00 UTC"

##

## $azimuth
## [1] 168.1455

##

## $elevation
## [1] 52.82587

##

## $diameter
## [1] 0.5246387

##

## $distance
## [1] 1.016318
```

The object to be supplied as argument for <code>geocode</code> is a data frame with variables <code>lon</code> and <code>lat</code>. This matches the return value of function <code>ggmap::geocode()</code>, function that can be used to find the coordinates using any 'address' entered as a character string understood by the Google maps API. We will not demonstrate this below, but all functions taking <code>lat</code> and <code>lon</code> arguments described can alternatively be supplied a geocode argument instead of separate latitude and longitude numeric values.

10.2 Times of sunrise, solar noon and sunset

Functions sunrise_time, sunset_time, noon_time, day_length and night_length have all the same parameter signature. In addition, function day_night returns a list containing all the quantities returned by the other functions. They are all vectorized for the date parameter.

We create a vector of dates to use in the examples—default time zone of ymd is UTC or GMT.

```
dates \leftarrow seq(from = ymd("2015-03-01"), to = ymd("2015-07-1"), length.out = 3)
```

Default latitude is zero (the Equator), the default longitude is zero (Greenwich), and default time zone for the functions in the photobiology package is "UTC". Be also aware that for summer dates the times are expressed accrodingly. In the examples below this can be recognized for example, by the time zone being reported as EEST instead of EET for Eastern Europe.

```
noon_time(dates, tz = "UTC", lat = 60)

## [1] "2015-03-01 12:12:48 UTC" "2015-05-01 11:57:17 UTC"

## [3] "2015-07-01 12:03:44 UTC"

noon_time(dates, tz = "CET", lat = 60)

## [1] "2015-03-01 13:12:48 CET" "2015-05-01 13:57:17 CEST"

## [3] "2015-07-01 14:03:44 CEST"
```

```
day_night(dates, lat = 60)

## $day

## [1] "2015-03-01" "2015-05-01" "2015-07-01"

##

## $sunrise

## [1] "2015-03-01 07:06:26 UTC" "2015-05-01 04:06:51 UTC"

## [3] "2015-07-01 02:52:50 UTC"

##

## $noon

## [1] "2015-03-01 12:12:48 UTC" "2015-05-01 11:57:17 UTC"

##

## $sunset

## [1] "2015-03-01 17:19:30 UTC" "2015-05-01 19:49:05 UTC"
```

```
## [3] "2015-07-01 21:14:09 UTC"
##
## $daylength
## [1] 10.21778 15.70382 18.35536
##
## $nightlength
## [1] 13.782215 8.296180 5.644636
```

The default for date is the current day.

```
sunrise_time(lat = 60)
## [1] "2015-12-13 09:04:52 UTC"
```

Both latitude and longitude can be supplied, but be aware that if the returned value is desired in the local time coordinates, the time zone should match the longitude.

```
sunrise_time(today(tzone = "UTC"), tz = "UTC", lat = 60, lon = 0)
## [1] "2015-12-13 09:04:52 UTC"
sunrise_time(today(tzone = "EET"), tz = "EET", lat = 60, lon = 25)
## [1] "2015-12-13 09:24:47 EET"
```

Southern hemisphere latitudes as well as longitudes to the West of the Greenwich meridian should be supplied as negative numbers.

```
sunrise_time(dates, lat = 60)

## [1] "2015-03-01 07:06:26 UTC" "2015-05-01 04:06:51 UTC"

## [3] "2015-07-01 02:52:50 UTC"

sunrise_time(dates, lat = -60)

## [1] "2015-03-01 05:18:13 UTC" "2015-05-01 07:47:52 UTC"

## [3] "2015-07-01 09:14:28 UTC"
```

The angle used in the twilight calculation can be supplied, either as the name of a standard definition, or as an angle in degrees (negative for sun positions below the horizon). Positive angles can be used when the time of sun occlusion behind a building, mountain, or other obstacle needs to be calculated.

Parameter unit.out can be used to obtain the returned value expressed as time-of-day in hours, minutes, or seconds since midnight.

Functions day_length and night_length return by default the length of time in hours.

```
day_length(dates, lat = 60)
## [1] 10.21778 15.70382 18.35536

night_length(dates, lat = 60)
## [1] 13.782215 8.296180 5.644636
```

Function day_night returns a list.

```
day_night(dates, lat = 60)
## $day
## [1] "2015-03-01" "2015-05-01" "2015-07-01"
## $sunrise
## [1] "2015-03-01 07:06:26 UTC" "2015-05-01 04:06:51 UTC"
## [3] "2015-07-01 02:52:50 UTC"
##
## $noon
## [1] "2015-03-01 12:12:48 UTC" "2015-05-01 11:57:17 UTC"
## [3] "2015-07-01 12:03:44 UTC"
##
## $sunset
## [1] "2015-03-01 17:19:30 UTC" "2015-05-01 19:49:05 UTC"
## [3] "2015-07-01 21:14:09 UTC"
## $daylength
## [1] 10.21778 15.70382 18.35536
##
## $nightlength
## [1] 13.782215 8.296180 5.644636
day_night(dates, lat = 60, unit.out = "hour")
## $day
## [1] "2015-03-01" "2015-05-01" "2015-07-01"
##
## $sunrise
```

```
## [1] 7.107340 4.114251 2.880713
##
## $noon
## [1] 12.21353 11.95495 12.06228
##
## $sunset
## [1] 17.32512 19.81807 21.23608
##
## $daylength
## [1] 10.21778 15.70382 18.35536
##
## $nightlength
## [1] 13.782215 8.296180 5.644636
```

11 RGB colours

Two functions allow calculation of simulated colour of light sources as R colour definitions. Three different functions are available, one for monochromatic light taking as argument wavelength values, and one for polychromatic light taking as argument spectral energy irradiances and the corresponding wave length values. The third function can be used to calculate a representative RGB colour for a band of the spectrum represented as a range of wavelength, based on the assumption of a flat energy irradiance across the range. By default CIE coordinates for *typical* human vision are used, but the functions have a parameter that can be used for supplying a different chromaticity definition.

Examples for monochromatic light:

```
w_length2rgb(550) # green

## wl.550.nm
## "#00FF00"

w_length2rgb(630) # red

## wl.630.nm
## "#FF0000"

w_length2rgb(c(550, 630, 380, 750)) # vectorized

## wl.550.nm wl.630.nm wl.380.nm wl.750.nm
## "#00FF00" "#FF0000" "#000000"
```

Examples for wavelength ranges:

```
w_length_range2rgb(c(400,700))
## 400-700 nm
## "#735B57"
```

Examples for spectra as vectors, in this case for the solar spectrum:

```
with(sun.spct, s_e_irrad2rgb(w.length, s.e.irrad))
## [1] "#544F4B"
with(sun.spct, s_e_irrad2rgb(w.length, s.e.irrad, sens = ciexyzCMF2.spct))
## [1] "#544F4B"
```

Examples with source_spct objects.

```
rgb_spct(sun.spct)
## [1] "#544F4B"

rgb_spct(sun.spct, sens = ciexyzCMF2.spct)
## [1] "#544F4B"
```

And also a color method for source_spct.

```
color(sun.spct)

## source CMF source CC
## "#544F4B" "#B63C37"

color(sun.spct * yellow.gel.spct)

## source CMF source CC
## "#946000" "#FF3B00"
```

12 Optimizing performance

When developing the current version of photobiology quite a lot of effort was spent in optimizing performance, especially of the functions accepting vectors as arguments, as in one of our experiments, we need to process several hundred thousands of measured spectra. The defaults should provide good performance in most cases, however, some further improvements are achievable, when a series of different calculations are done on the same spectrum, or when a series of spectra measured at exactly the same wavelengths are used for calculating weighted irradiances or exposures.

In the case of doing calculations repeatedly on the same spectrum, a small improvement in performance can be achieved by setting the parameter check.spectrum = FALSE for all but the first call to irradiance(), or photon_irradiance(), or energy_irradiance(), or the equivalent function for ratios. It is also possible to set this parameter to FALSE in all calls, and do the check beforehand by explicitly calling check_spectrum().

In the case of calculating weighted irradiances on many spectra having exactly the same wavelength values, then a significant improvement in the performance can be achieved by setting use.cached.mult = TRUE, as this reuses

Table 12: Data sets included in the package: spectra. The CIE standard illuminant data in this package are normalized to one at $\lambda=560\,\mathrm{nm}$, while in the CIE standard they are normalized to 100 at the same wavelength.

Object	class	units	data description
<pre>sun.spct sun.daily.spct sun.data sun.daily.data D65.illuminant.spct A.illuminant.spct</pre>	source_spct source_spct data.frame data.frame source_spct source_spct	$\begin{array}{c} Wm^{-2}nm^{-1} \\ Jm^{-2}d^{-1}nm^{-1} \\ Wm^{-2}nm^{-1} \\ Jm^{-2}d^{-1}nm^{-1} \\ (norm.\ 560\ nm) \\ (norm.\ 560\ nm) \end{array}$	solar spectral irradiance solar spectral exposure solar spectral irradiance solar spectral exposure CIE standard CIE standard

Table 13: Data sets included in the package: chromaticity data

Object	class	data description
ciexyzCC2.spct ciexyzCC10.spct ciexyzCMF2.spct ciexyzCMF10.spct ciev2.spct ciev10.spct beesxyzCMF.spct	chroma_spct chroma_spct chroma_spct chroma_spct chroma_spct chroma_spct	human chromaticity coordinates 2° human chromaticity coordinates 10° human colour matching function 2° human colour matching function 10° human luminous efficiency 2° human luminous efficiency 10° bee colour matching function

the multipliers calculated during successive calls based on the same waveband. However, to achieve this increase in performance, the tests to ensure that the wavelength values have not changed, have to be kept to the minimum. Currently only the length of the wavelength array is checked, and the cached values discarded and recalculated if the length changes. For this reason, this is not the default, and when using caching the user is responsible for making sure that the array of wavelengths has not changed between calls.

You can use the package microbenchmark to time the code and find the parts that slow it down. I have used it, and also I have used profiling to optimize the code for speed. The choice of defaults is based on what is best when processing a moderate number of spectra, say less than a few hundreds, as opposed to many thousands.

13 Example data

A few example spectra are included in this package for use in examples and vignettes, and testing (Tables 12 and 13).