photobiology Version 0.3.10 User Guide

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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 (photobiologyUV), visible radiation (photobiologyVIS), or based on Phytochrome (photobiologyPhy), Cryptochrome (photobiologyCry) (both photoreceptors present in plants), and spectral data for filters (photobiologyFilters). In the future it will be submitted to CRAN (Comprehensive R archive network), it is meanwhile available from https://bitbucket.org/aphalo/photobiology/downloads. There is also a public Git repository at https://bitbucket.org/aphalo/photobiology from where the source code of the current an earlier versions can be cloned.

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(photobiologyWavebands)
library(photobiologyFilters)
library(ggplot2)
library(ggtern)
```

3 Data formats

The package 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 every-day 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.

3.1 Example spectral data

A few data objects are included in the package for use in examples. Two simulated solar spectra, sun.spct and sun.daily.spct, ...

3.2 Using numeric vectors

When dealing with spectra, we operate on pairs of vectors, one with the wavelengths in nm, and a second one with the corresponding values for the spectral data.

It is usual to 'group' these two (or more) vectors into a data frame. For vectors within a data frame we need to 'make them visible' when operating with the functions that expect numeric vectors as arguments.

3.3 Using 'spectra' objects

This package defines a family of objects based on data tables (data frame compatible objects) which impose some restrictions on the naming of the vectors, something that allows the second set of 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 derived from data.table objects, which in turn are derived from data.frame objects. In this package we define a generic spectrum type of object, derived from data table, from which specialized types of spectra are derived. This 'parenthood' hierarchy means that spectra objects can be used almost anywhere where a data.frame or data.table is expected. Many functions defined in package data.table and useful when working with spectra are re-exported by the current package, so that in most cases there is no need to explicitly include library(data.table) in your scripts.

Although data.tables are syntactically compatible with data.frames, in some special cases the same code may have different semantics as data tables use references in some cases were data frames would use a copy of the data. In general, no such problems exist, and the different semantics only applies to data table specific syntax. If in doubt, to avoid problems, when you really intend to make a new copy of a spectrum, preserving the original object unchanged by later operations on the new 'name', use function copy in addition to the assignment operator.

```
# 1) data frame syntax on a data.frame
a.df <- data.frame(x=1:3, y=rep(1, 3))
b.df <- a.df
b.df$y <- b.df$y * 2
b.df
## x y
## 1 1 2
## 2 2 2
## 3 3 2
a.df # not modified!
## x y
## 1 1 1
## 2 2 1
## 3 3 1
# 2) data frame syntax on a data.table
a.dt <- data.table(x=1:3, y=rep(1, 3))
b.dt <- a.dt
b.dt$y <- b.dt$y * 2
b.dt
## x y
## 1: 1 2
## 2: 2 2
## 3: 3 2
a.dt # not modified!
## x y
## 1: 1 1
## 2: 2 1
## 3: 3 1
# 3) data table syntax on a data.table
a.dt <- data.table(x=1:3, y=rep(1, 3))
b.dt <- a.dt
b.dt[ , y := y * 2]
## x y
## 1: 1 2
## 2: 2 2
## 3: 3 2
a.dt # modified!
## x y
## 1: 1 2
## 2: 2 2
## 3: 3 2
# 4) forcing creation of a copy
a.dt <- data.table(x=1:3, y=rep(1, 3))
c.dt <- copy(a.dt)</pre>
c.dt[, y := y * 2]
```

From the examples above one can see that in example 3) b.dt is not a copy of a.dt, but instead a reference (a new name pointing to the original object), while in examples 1), 2) and 4) b.dt, is a new object, initialized to the value of a.dt.

3.4 Spectral 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. Ånstrom (1 Å = $1 \cdot 10^{-10}$ m), the values need to be rescaled before any calculations. Not doing so will yield completely wrong results!

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.

If our spectral irradiance data is in W m⁻² nm⁻¹, and the wavelength in nm, as in the case of Macam spectroradiometers, the data can be used directly and functions in the package will return irradiances in W m⁻².

If, for example, the spectral irradiance output by our model of spectroradiometer is in $\rm mW\,m^{-2}\,nm^{-1}$, and the wavelengths are in Ångstrom then to obtain the effective irradiance in $\rm W\,m^{-2}$ we will need to rescale the data.

```
# not run
energy_irradiance(wavelength/10, irrad/1000)
```

In the example above, we take advantage of the behavior 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.

It is very 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.

3.5 Creation

generic.spct objects can be created from data tables and data frames simply by setting them as such. However, a column called w.length must be present and contain wavelength values expressed in nm.

```
a.spct <- setGenSpct(data.table(w.length = 300:305, y = rep(1,6)))</pre>
class(a.spct)
## [1] "generic.spct" "data.table"
                                      "data.frame"
a.spct
##
    w.length y
## 1:
           300 1
## 2:
           301 1
## 3:
           302 1
## 4:
           303 1
           304 1
## 5:
           305 1
## 6:
```

<code>source.spct</code> objects can be created from data tables, data frames, and <code>generic.spct</code> simply by setting them as such. However, a columns called <code>w.length</code> (wavelength values expressed in nm) and <code>s.e.irrad</code> (W m $^{-2}$ nm $^{-1}$) and \or s.q.irrad (mol m $^{-2}$ s $^{-1}$ nm $^{-1}$) must be present.

```
b.spct <- setSourceSpct(data.table(w.length = 300:305, s.e.irrad = rep(1,6)))</pre>
class(b.spct)
## [1] "source.spct" "generic.spct" "data.table"
                                                      "data.frame"
b.spct
##
     w.length s.e.irrad
## 1:
           300
                      1
## 2:
           301
## 3:
           302
                       1
           303
## 4:
                       1
## 5:
           304
                       1
## 6:
           305
                       1
```

If the spectral irradiance is expressed per day, then the parameter time.unit should be set to "day" instead of the default of "second". This information can be used when printing the results.

```
b.d.spct <- setSourceSpct(
   data.table(w.length = 300:305, s.e.irrad = rep(1,6)),
   time.unit="day")
attr(b.d.spct, "time.unit")
## [1] "day"
class(b.d.spct)
## [1] "source.spct" "generic.spct" "data.table" "data.frame"</pre>
```

```
b.d.spct
##
      w.length s.e.irrad
## 1:
           300
                        1
## 2:
           301
                        1
## 3:
           302
## 4:
           303
                        1
## 5:
           304
                        1
## 6:
           305
```

filter.spct objects can be created from data tables, data frames, and generic.spct simply by setting them as such. However, columns called w.length (wavelength values expressed in nm) and Tpc (T%), Tfr (T as fraction of 1) and $\$ (absorbance (\log_{10} based)) must be present.

```
c.spct <- setFilterSpct(data.table(w.length = 300:305, Tfr = rep(1,6)))</pre>
class(c.spct)
## [1] "filter.spct" "generic.spct" "data.table"
                                                    "data.frame"
c.spct
##
     w.length Tfr
## 1:
           300 1
## 2:
           301
                1
## 3:
           302 1
## 4:
           303 1
           304
               1
## 5:
## 6:
           305
```

reflector.spct objects can be created from data tables, data frames, and generic.spct simply by setting them as such. However, columns called w.length (wavelength values expressed in nm) and Rpc (R%), and or Rfr (R as fraction of 1) must be present.

```
d.spct <- setReflectorSpct(data.table(w.length = 300:305, Rfr = rep(1,6)))</pre>
class(d.spct)
## [1] "reflector.spct" "generic.spct"
                                          "data.table"
                                                           "data.frame"
d.spct
##
      w.length Rfr
## 1:
           300 1
## 2:
           301
                 1
## 3:
           302
                1
## 4:
           303 1
## 5:
           304
                1
           305
## 6:
```

<code>chroma.spct</code> objects can be created from data tables, data frames, and <code>generic.spct</code> simply by setting them as such. However, columns called <code>w.length</code> (wavelength values expressed in nm) and x, y and z must be present, giving the trichromic chromaticity constants.

```
e.spct <- setChromaSpct(data.table(w.length = 300:305, x = rep(1,6), y = rep(1,6), z = rep(1,6)))
class(e.spct)
## [1] "chroma.spct" "generic.spct" "data.table"
e.spct
##
    w.length x y z
## 1:
          300 1 1 1
## 2:
           301 1 1 1
## 3:
           302 1 1 1
## 4:
           303 1 1 1
## 5:
          304 1 1 1
        305 1 1 1
## 6:
```

In all cases if the expected data is not available, then it is filled in if possible with values, and if not with NAs.

```
f.spct <- setReflectorSpct(data.table(w.length = 300:305, Rpc = rep(100,6)))</pre>
class(f.spct)
## [1] "reflector.spct" "generic.spct" "data.table"
                                                        "data.frame"
f.spct
##
     w.length Rpc Rfr
## 1:
        300 100
## 2:
          301 100 1
          302 100 1
## 3:
## 4:
          303 100
                   1
## 5:
          304 100
                    1
        305 100 1
## 6:
```

When required data is not available, and it cannot be calculated from other columns, the required column is added and filled with NAs.

```
g.spct <- setReflectorSpct(data.table(w.length = 300:305, z = rep(1,6)))</pre>
## Warning: No reflectance data found in filter.spct
class(g.spct)
## [1] "reflector.spct" "generic.spct" "data.table"
                                                          "data.frame"
g.spct
     w.length z Rfr
##
         300 1 NA
## 1:
## 2:
           301 1 NA
## 3:
           302 1 NA
## 4:
           303 1 NA
## 5:
           304 1 NA
## 6:
          305 1 NA
```

If no ${\tt w.length}$ column is present, and a ${\tt wl}$ column is found, it is renamed to ${\tt w.length}$.

```
h.spct <- setReflectorSpct(data.table(wl = 300:305, Rfr = rep(1,6)))
class(h.spct)
## [1] "reflector.spct" "generic.spct"
                                        "data.table"
                                                         "data.frame"
h.spct
##
     w.length Rfr
          300 1
## 1:
## 2:
          301
               1
## 3:
          302
## 4:
          303 1
## 5:
          304
               1
## 6:
          305
               1
```

Here we just use the example data supplied with the package.

```
class(sun.spct)
## [1] "source.spct" "generic.spct" "data.table"
                                                  "data.frame"
sun.spct
##
       w.length s.e.irrad s.q.irrad
        293 2.610e-06 6.392e-12
##
   1:
##
    2:
            294 6.142e-06 1.510e-11
## 3:
            295 2.176e-05 5.366e-11
##
           296 6.780e-05 1.678e-10
  4:
## 5:
          297 1.533e-04 3.807e-10
## ---
## 504:
            796 4.081e-01 2.715e-06
            797 4.141e-01 2.759e-06
## 505:
            798 4.236e-01 2.826e-06
## 506:
            799 4.186e-01 2.796e-06
## 507:
## 508:
          800 4.069e-01 2.721e-06
```

3.6 Conversions

The functions e2q and q2e can be used on source spectra to convert spectral energy irradiance into spectral photon irradiance and vice versa. The first argument should be a spectrum, and the second optional argument sets the action with "add" and "replace" as possible values. In the second case the whole spectrum object is copied, while in the first case a column is added but the unchanged columns are references to the original ones, rather than copies.

```
b.spct
##
      w.length s.e.irrad
## 1:
           300
                      1
## 2:
           301
                       1
## 3:
           302
                        1
## 4:
           303
                        1
## 5:
           304
                        1
## 6:
           305
```

```
b1.spct <- e2q(b.spct, "replace")
b.spct
##
     w.length s.e.irrad
        300
## 1:
                     1
## 2:
          301
## 3:
          302
## 4:
          303
                      1
## 5:
          304
## 6:
          305
                      1
b1.spct
##
     w.length s.q.irrad
## 1:
          300 2.508e-06
## 2:
          301 2.516e-06
## 3:
          302 2.524e-06
## 4:
          303 2.533e-06
## 5:
          304 2.541e-06
## 6:
          305 2.550e-06
b2.spct <- e2q(b.spct, "add")
b.spct
##
     w.length s.e.irrad
## 1:
          300
                     1
## 2:
          301
                      1
## 3:
          302
## 4:
          303
                      1
## 5:
          304
## 6:
          305
                      1
b2.spct
##
     w.length s.e.irrad s.q.irrad
          300 1 2.508e-06
301 1 2.516e-06
## 1:
## 2:
## 3:
          302
                     1 2.524e-06
## 4:
          303
                     1 2.533e-06
          304
## 5:
                      1 2.541e-06
## 6:
          305
                     1 2.550e-06
```

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

3.7 Remapping a spectrum to different wavelengths

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 new wavelengths.

3.8 Summaries

Functions integrate_spct and average_spct take into account each individual wavelength step, so they return valid results even for spectra measured at arbitrary and varying wavelength steps.

```
integrate_spct(sum.spct)

## e.irrad q.irrad
## 2.691e+02 1.255e-03

average_spct(sum.spct)

## e.irrad q.irrad
## 5.308e-01 2.476e-06
```

'Normal' and a couple of new functions are also available for spectra, but redefined to return wavelengths.

```
range(sum.spct)
## [1] 293 800
min(sum.spct)
## [1] 293
max(sum.spct)
## [1] 800
midpoint(sum.spct)
## [1] 546.5
spread(sum.spct)
## [1] 507
```

Method definitions for summary and 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 with using the correct units.

```
## wavelength ranges from 293 to 800 nm
## largest wavelength step size is 1 nm
## spectral irradiance ranges from 2.61e-06 to 0.8205 W m-2 nm-1
## energy irradiance is 269.1 W m-2
## photon irradiance is 1255 umol s-1 m-2
```

```
## wavelength ranges from 290 to 800 nm
## largest wavelength step size is 1 nm
## spectral irradiance ranges from 0 to 32.61 kJ d-1 m-2 nm-1
## energy irradiance is 10.93 MJ m-2
## photon irradiance is 51.39 mol d-1 m-2
```

4 Using operators with spectra

The basic math 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.

```
sun.spct / sun.spct
      w.length s.e.irrad
## 1: 293 1
## 2:
           294
## 3: 295
## 4: 296
## 5: 297
                     1
## ---
## 504: 796
## 505: 797
                     1
                      1
## 506:
## 507:
## 508:
           798
                      1
           799
                      1
           800
                      1
sun.spct + sun.spct
##
      w.length s.e.irrad
## 1: 293 5.219e-06
## 2: 294 1.228e-05
## 3: 295 4.352e-05
## 4: 296 1.356e-04
## 5:
          297 3.067e-04
## ---
## 504: 796 8.161e-01
```

```
## 505: 797 8.282e-01
## 506: 798 8.473e-01
## 507: 799 8.372e-01
## 508: 800 8.138e-01
```

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

```
sun.spct * 2
##
        w.length s.e.irrad
##
    1:
             293 5.219e-06
##
    2:
             294 1.228e-05
##
    3:
             295 4.352e-05
##
    4:
             296 1.356e-04
##
    5:
             297 3.067e-04
##
## 504·
             796 8.161e-01
## 505:
             797 8.282e-01
## 506:
             798 8.473e-01
             799 8.372e-01
## 507:
## 508:
             800 8.138e-01
sun.spct * c(0,1)
##
        w.length s.e.irrad
##
    1:
            293 0.000e+00
##
    2:
             294 6.142e-06
##
    3:
             295 0.000e+00
##
     4:
             296 6.780e-05
##
    5:
             297 0.000e+00
## 504:
             796 4.081e-01
## 505:
             797 0.000e+00
## 506:
             798 4.236e-01
## 507:
             799 0.000e+00
## 508:
```

There is one special case, for chroma.spct: if the second operand is a numeric vector of length three, containing three named values 'x', 'y' and 'z', the corresponding element is used for each of the chromaticity 'columns' in the chroma.spct. Un-named values or differently named values are not treated specially.

5 Defining wavebands

All functions use wavebands as definitions of the range of wave lengths and the spectral weighting function (SWF) to use in the calculations. A few other bits of information may 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. Waveband objects belong to the S3 class "waveband".

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.

6 Calculating irradiance or exposure

There is one basic function for these calculations <code>irradiance()</code>, it 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 <code>unit.in</code> cab be used to adjust the calculations to expect photon units. The type of unit used for the calculated irradiance (or exposure) is set by the parameter <code>unit.out</code> with no default. If no <code>w.band</code> parameter is supplied, the whole spectrum spectrum input is used, unweighted, to calculate the total irradiance. If a <code>w.band</code> is supplied, then the range of wavelengths specified and SWF if present are used for calculating the irradiance. If the waveband definition does not include a SWF, then the unweighted irradiance is returned, if the definition includes a SWF, then a weighted irradiance is returned.

The functions photon_irradiance() and energy_irradiance(), just call irradiance() with the unit.out set to "photon" or "energy" respectively.

Then we compare the calculations based on the different wavebands defined in the previous section and the predefined functions in the packages photobiologyUS and photobiologyUV. The predefined functions have the advantage of allowing the specification of parameters to modify the w.band created. In the example bellow, we use this to set the normalization wavelength.

This is how CIE() is defined in photobiologyUV.

```
wb.name=paste("CIE98", as.character(norm), sep="."))
}
```

The generic functions print(), min(), max(), range(), midpoint() and labels() call the corresponding special functions defined for waveband objects: print.waveband(), range.waveband(), etc.

```
PAR()
## PAR
## low (nm) 400
## high (nm) 700
## weighted none
str(PAR())
## List of 10
## $ low
           : num 400
## $ high
            : num 700
## $ weight : chr "none"
## $ SWF.e.fun: NULL
## $ SWF.q.fun: NULL
## $ SWF.norm : NULL
## $ norm : NULL
## $ hinges : num [1:4] 400 400 700 700
## $ name : chr "PAR" ## $ label : chr "PAR"
## - attr(*, "class")= chr [1:2] "waveband" "list"
range(PAR())
## [1] 400 700
spread(PAR())
## [1] 300
min(PAR())
## [1] 400
max(PAR())
## [1] 700
midpoint(PAR()) # gives wavelength at center
## [1] 550
normalization(PAR())
## [1] NA
color(PAR()) # equivalent RGB color definitions
## PAR CMF PAR CC
## "#735B57" "#8D4C3D"
labels(PAR())
## $label
## [1] "PAR"
##
## $name
## [1] "PAR"
```

```
CIE()
## CIE98.298
## low (nm) 250
## high (nm) 400
## weighted SWF
## normalized at 298 nm
str(CIE())
## List of 10
## $ low : num 250
## $ high : num 400
## $ weight : chr "SWF"
## $ SWF.e.fun:function (w.length)
## $ SWF.q.fun:function (w.length)
## $ SWF.norm : num 298
## $ norm : num 298
## $ hinges : num [1:6] 250 250 298 328 400 ...
## $ name : chr "CIE98.298"
## $ label : chr "CIE98"
## - attr(*, "class")= chr [1:2] "waveband" "list"
labels(CIE())
## $label
## [1] "CIE98"
##
## $name
## [1] "CIE98.298"
labels(CIE(300))
## $label
## [1] "CIE98"
##
## $name
## [1] "CIE98.300"
normalization(CIE())
## [1] 298
normalization(CIE(300))
## [1] 300
labels(UVB())
## $label
## [1] "UVB"
##
## $name
## [1] "UVB.ISO"
labels(UVB("medical"))
```

```
## $label
## [1] "UVB"
##
## $name
## [1] "UVB.medical"

labels(UVB("ISO"))

## $label
## [1] "UVB"
##
## ## $name
## [1] "UVB.ISO"
```

```
labels(new_waveband(100, 200))
## $label
## [1] "range.100.200"
##
## $name
## [1] "range.100.200"
labels(new_waveband(100, 200, wb.name="ANY NAME"))
## $label
## [1] "ANY NAME"
##
## $name
## [1] "ANY NAME"
labels(new_waveband(100, 200, wb.name="ANY SHORT NAME",
                    wb.label="ANY LONG LABEL"))
## $label
## [1] "ANY LONG LABEL"
##
## $name
## [1] "ANY SHORT NAME"
```

6.1 Irradiances from vectors

Here we describe the functions that use vectors as arguments. In the next section we describe similar functions for spct objects.

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

```
with(sun.data, photon_irradiance(w.length, s.e.irrad, PAR()))
## PAR
## 0.0008938
with(sun.spct, photon_irradiance(w.length, s.e.irrad, PAR()))
## PAR
## 0.0008938
```

The recommended practice is to use with, as above. But to keep code lines shorter and simpler we attach the data frame sun.data to make the contained vectors visible. The use of w.length and s.e.irrad and 7 or s.q.irrad is just our convention, and vectors of any name can be supplied as arguments.

```
attach(sun.data)
```

Some examples comparing different definitions of wavebands for PAR. Photon irradiance is expressed in $\text{mol m}^{-2} \, \text{s}^{-1}$.

```
photon_irradiance(w.length, s.e.irrad, my_PAR)

## range.400.700
## 0.0008938

photon_irradiance(w.length, s.e.irrad, my_PARx)

## my_PARx
## 0.0008938

photon_irradiance(w.length, s.e.irrad, PAR())

## PAR
## 0.0008938

photon_irradiance(w.length, s.e.irrad, PAR()) * 1e6

## PAR
## 893.8
```

Some examples comparing different definitions of wavebands for erythemal UV-B (CIE98) irradiance in W $\rm m^{-2}$.

```
photon_irradiance(w.length, s.e.irrad, my_CIE_1)

## range.250.400.wtd
## 2.037e-07

photon_irradiance(w.length, s.e.irrad, my_CIE_2)

## range.250.400.wtd
## 2.037e-07

photon_irradiance(w.length, s.e.irrad, my_CIE_3)

## range.250.400.wtd
## 2.037e-07

energy_irradiance(w.length, s.e.irrad, my_CIE_1)

## range.250.400.wtd
## 0.08178

energy_irradiance(w.length, s.e.irrad, my_CIE_2)
```

Lists of wavebands are also accepted as argument.

```
energy_irradiance(w.length, s.e.irrad, list(CIE(), CIE(298), CIE(300)))

## CIE98.298 CIE98.298 CIE98.300
## 0.08178 0.08178 0.12608

my_wavebands <- list(Red(), Blue(), Green())
energy_irradiance(w.length, s.e.irrad, my_wavebands)

## Red.ISO Blue.ISO Green.ISO
## 79.61 37.58 49.30</pre>
```

The are also convenience functions for calculating how 'total' irradiance is split among different contiguous bands of the spectrum. The functions split_photon_irradiance() and split_energy_irradiance(), just call split_irradiance() with the unit.out set to "photon" or "energy" respectively.

Now we detach the data frame.

```
detach(sun.data)
```

6.2 Irradiances from spectra

The code using spct objects is much simpler.

```
e_irrad_spct(sun.spct, PAR())

## PAR
## 196.7

q_irrad_spct(sun.spct, PAR())

## PAR
## 0.0008938
```

7 Calculating ratios

7.1 Ratios from 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 'ratio' functions in the photobiology package.

The derived functions are: photon_ratio(), energy_ratio(), and photons_energy_ratio. The packages photobiologyVIS and photobiologyUV use these to define some convenience functions, and here we give and example for a function not yet implemented, but which you may find as a useful example.

If for example we would like to calculate the ratio between UVB and PAR radiation, we would use either of the following function calls, depending on which type of units we desire.

We attach again the data frame.

```
attach(sun.data)

photon_ratio(w.length, s.e.irrad, UVB(), PAR())

## [1] 0.001708

energy_ratio(w.length, s.e.irrad, UVB(), PAR())

## [1] 0.00299
```

If we would like to calculate a conversion factor between PPFD (PAR photon irradiance in mol s-1 m-2) and PAR (energy) irradiance (W m-2) for a light source for which we have spectral data we could use the following code.

```
conv.factor <- photons_energy_ratio(w.length, s.e.irrad, PAR())

PPFD.mol.photon <- 1000e-6
PAR.energy <- PPFD.mol.photon / conv.factor
print(conv.factor)

## [1] 4.544e-06

print(PPFD.mol.photon * 1e6)

## [1] 1000
print(PAR.energy)

## [1] 220.1</pre>
```

The 'ratio' functions do not accept lists of waveband objects as the 'irradiance' functions do. This is a feature, as otherwise it would be too easy to make mistakes. It is possible to use the 'irradiance' functions to calculate several ratios in one go.

7.2 Ratios from spectra

```
qe_ratio_spct(sun.spct, PAR())
## q:e(PAR)
## 4.544e-06

qe_ratio_spct(sun.spct, list(Blue(), Green(), Red()))
## q:e(Blue.ISO) q:e(Green.ISO) q:e(Red.ISO)
## 3.964e-06 4.465e-06 5.680e-06
```

7.3 Tagging observations in a spectrum

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

```
tag(sun.spct, PAR(), byref=FALSE)
##
       w.length s.e.irrad s.q.irrad wl.color wb.color wb.name wb.f
  1: 293 2.610e-06 6.392e-12 #000000 NA none none
           294 6.142e-06 1.510e-11 #000000
                                               NA none none
## 2:
          295 2.176e-05 5.366e-11 #000000
296 6.780e-05 1.678e-10 #000000
                                               NA none none
##
    3:
##
    4:
          297 1.533e-04 3.807e-10 #000000
## 5:
                                               NA none none
## 504:
           796 4.081e-01 2.715e-06 #000000
                                               NA none none
                                               NA
## 505:
            797 4.141e-01 2.759e-06 #000000
                                                     none none
## 506:
           798 4.236e-01 2.826e-06 #000000
                                                NA
                                                     none none
## 507:
           799 4.186e-01 2.796e-06 #000000
                                               NA none none
## 508:
          800 4.069e-01 2.721e-06 #000000
                                               NA none none
tag(sun.spct, UV_bands(), byref=FALSE)
```

```
##
       w.length s.e.irrad s.q.irrad wl.color wb.color wb.name wb.f
##
            293 2.610e-06 6.392e-12 #000000 #000000
    1:
##
    2:
            294 6.142e-06 1.510e-11 #000000
                                             #000000
    3:
##
            295 2.176e-05 5.366e-11 #000000 #000000
                                                        UVB UVB
    4:
            296 6.780e-05 1.678e-10 #000000 #000000
                                                        UVB UVB
##
   5:
            297 1.533e-04 3.807e-10 #000000 #000000
                                                        UVB UVB
##
## 504:
            796 4.081e-01 2.715e-06 #000000
                                                       none none
            797 4.141e-01 2.759e-06 #000000
## 505:
                                                  NΑ
                                                       none none
            798 4.236e-01 2.826e-06 #000000
## 506:
                                                  NA
                                                       none none
## 507:
            799 4.186e-01 2.796e-06 #000000
                                                  NA
                                                       none none
## 508:
            800 4.069e-01 2.721e-06 #000000
                                                 NA
                                                      none none
```

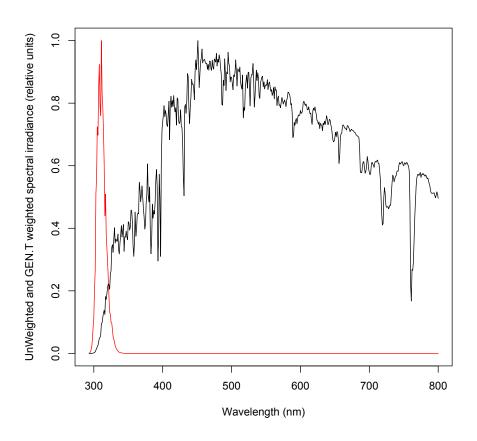
The added factor, labels, and colour data can be used for further processing or for plotting.

8 Calculating weighted spectral irradiances

This calculation is not very frequently used, but it is very instructive to look at spectral data in this way, as it can make apparent the large effect that small measuring errors can have on the estimated effective irradiances or exposures.

8.1 Weighted spectral irradiance from vectors

We here plot weighted and unweighted irradiances using simulated solar spectral irradiance data.



8.2 Weighted spectral irradiance from an unweighted source spectrum

The multiplication operator is defined for operation between a source.spct and a waveband.

```
sun.CIE.spct <- sun.spct * CIE()</pre>
sun.CIE.spct
##
        w.length s.e.irrad
##
     1:
             293 2.610e-06
##
     2:
             294 6.142e-06
##
     3:
             295 2.176e-05
##
     4:
             296 6.780e-05
##
     5:
             297 1.533e-04
##
## 504:
             796 0.000e+00
## 505:
             797 0.000e+00
```

```
## 506: 798 0.000e+00
## 507: 799 0.000e+00
## 508: 800 0.000e+00
```

9 Position of the sun in the sky

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 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] "2014-08-14 00:11:14 EEST"
##
## $azimuth
## [1] 312.1
##
## $elevation
## [1] -26.32
## $diameter
## [1] 0.5263
##
## $distance
## [1] 1.013
sun_angles(ymd_hms("2014-01-01 0:0:0", tz="UTC"))
## $time
## [1] "2014-01-01 UTC"
##
## $azimuth
## [1] 182
##
## $elevation
## [1] -66.96
##
## $diameter
## [1] 0.5423
## $distance
## [1] 0.9833
```

10 Calculating times of sunrise and sunset

```
day_night()
## $day
## [1] "2014-08-14 EEST"
## $sunrise
## [1] "2014-08-14 09:04:44 EEST"
##
## $noon
## [1] "2014-08-14 15:04:34 EEST"
##
## $sunset
## [1] "2014-08-14 21:04:38 EEST"
##
## $daylength
## Time difference of 12 hours
## $nightlength
## Time difference of 12 hours
day_night(ymd("2014-05-30", tz = "UTC"), lat=30, lon=0)
## $day
## [1] "2014-05-30 UTC"
##
## $sunrise
## [1] "2014-05-30 08:04:12 EEST"
## $noon
## [1] "2014-05-30 14:57:32 EEST"
##
## $sunset
## [1] "2014-05-30 21:51:05 EEST"
## $daylength
## Time difference of 13.78 hours
##
## $nightlength
## Time difference of 10.22 hours
day_night(ymd("2014-05-30", tz = "UTC"), lat=30, lon=0, twilight="civil")
## $day
## [1] "2014-05-30 UTC"
##
## $sunrise
## [1] "2014-05-30 08:34:25 EEST"
## $noon
## [1] "2014-05-30 14:57:32 EEST"
## $sunset
## [1] "2014-05-30 21:20:49 EEST"
##
## $daylength
## Time difference of 12.77 hours
## $nightlength
## Time difference of 11.23 hours
```

11 Calculating equivalent RGB colours for display

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
     550 nm
## "#00FF00"
w_length2rgb(630) # red
     630 nm
## "#FF0000"
w_length2rgb(380) # UVA
     380 nm
## "#000000"
w_length2rgb(750) # far red
     750 nm
## "#000000"
w_length2rgb(c(550, 630, 380, 750)) # vectorized
     550 nm
               630 nm
                          380 nm
                                    750 nm
## "#00FF00" "#FF0000" "#000000" "#000000"
```

Examples for wavelength ranges:

```
w_length_range2rgb(c(400,700))

## 400-700 nm
## "#735B57"

w_length_range2rgb(400:700)

## Warning: Using only extreme wavelength values.

## 400-700 nm
## "#735B57"
```

```
w_length_range2rgb(sun.spct$w.length)

## Warning: Using only extreme wavelength values.

## 293-800 nm
## "#554340"

w_length_range2rgb(550)

## Warning: Calculating RGB values for monochromatic light.

## 550 nm
## "#00FF00"
```

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"
with(sun.spct, s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCMF10.spct))
## [1] "#59534F"
with(sun.spct, s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCC2.spct))
## [1] "#B63C37"
with(sun.spct, s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCC10.spct))
## [1] "#BD3C33"
```

Examples with source.spct objects.

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

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

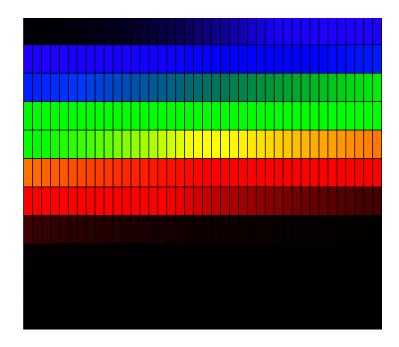
And also a color method for source.spct.

```
color(sun.spct)
## source CMF source CC
## "#544F4B" "#B63C37"

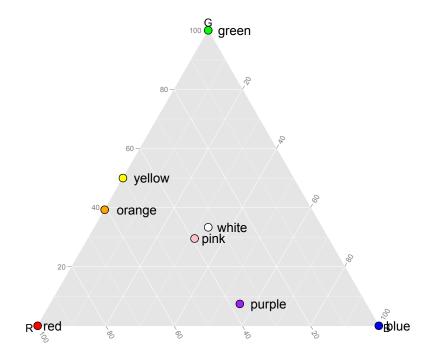
color(sun.spct * rg630.spct)
## source CMF source CC
## "#4A0000" "#FF0000"
```

Here we plot the RGB colours for the range covered by the CIE 2006 proposed standard calculated at each 1 nm step: $\frac{1}{2}$

RGB colours for 390 to 829 nm



Given a color in any of the above ways, yields RGB values that can be used to locate the position of any colour on Maxwell's triangle. Here using R's predefined colours.

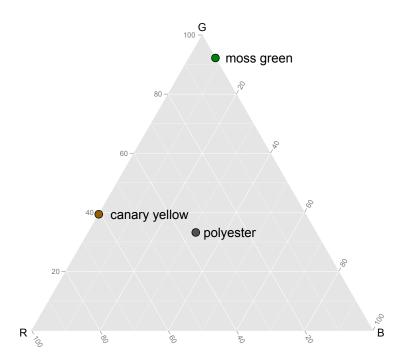


We simulate the spectra of filtered sunlight by multiplying the solar spectrum by filter transmittance spectra.

```
yellow.light.spct <- canary.yellow.new.spct * sun.spct
green.light.spct <- moss.green.new.spct * sun.spct
polyester.light.spct <- polyester.new.spct * sun.spct</pre>
```

Now using the filtered sunlight spectra we calculate colours based on human vision photoreceptors.

```
aes(x=R, y=G, z=B, fill=colour, label=labels)) +
geom_point(shape=21, size=4) +
geom_text(hjust=-0.15) +
labs(x = "R", y="G", z="B") +
scale_fill_identity()
maxwell.tern
```



12 Auxiliary functions

Sometimes it is needed to add (parallel sum) between two spectra, even if the two spectra have been measured at different wavelengths or wavelength steps. This can happen for example when we would like to calculate the spectrum of a combination of two light sources from the individual spectra. The function sum_spectra() can be used in such a case. It's use is described in User Guide of the photobiologyLamps package.

A function interpolate_spectrum is also included to facilitate interpolation

of spectral values. It is used in the function described in the previous paragraph, but also be used by itself when interpolation is needed. Under the hood it uses R's spline function if there are fewer than 25 data points, and uses approx otherwise. It allows easier control of values to be used for extrapolation.

13 Dealing with real 'noisy' spectral data

The first thing to do is to think whether any part of the spectral measurements can be *a priori* known to be equal to zero. For example for the solar spectrum at ground level it is safe to assume that the spectral irradiance is zero for all wavelengths shorter than 293 nm. If the data are noisy, it is best to discard these data before calculating any effective UV doses.

In the following example we use a longer wavelength (297 nm) just to show how the function works, because the example spectral data set starts at 293 nm.

```
head(sun.spct)

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

## 1:     293     2.610e-06     6.392e-12

## 2:     294     6.142e-06     1.510e-11

## 3:     295     2.176e-05     5.366e-11

## 4:     296     6.780e-05     1.678e-10

## 5:     297     1.533e-04     3.807e-10

## 6:     298     3.670e-04     9.141e-10
```

Sub-setting can be easily done as follows if the data are in a data.frame (of course, replacing w.length with the name used in your data frame for the wavelengths array):

```
subsetted.sun.spct <- subset(sun.spct, w.length >= 297)
head(subsetted.sun.spct)
##
     w.length s.e.irrad s.q.irrad
## 1:
           297 0.0001533 3.807e-10
## 2:
           298 0.0003670 9.141e-10
## 3:
           299 0.0007845 1.961e-09
## 4:
           300 0.0012646 3.171e-09
## 5:
           301 0.0026237 6.602e-09
## 6:
           302 0.0039226 9.903e-09
```

And then just use the sub-setted data in your calculations.

If the data are not in a dataframe, then there are different options: 1) create a data frame from your data, 2) use the function trim_tails() from this package, or 3) just use R commands. Here we give examples of the use of trim_tails(), and just use the same data as in earlier examples. First we delete all data for wavelengths shorter than 293 nm.

13.1 Trimming spectra stored as vectors

```
trimmed.sun.spct <-</pre>
 trim_tails(w.length, s.e.irrad, low.limit=297)
head(trimmed.sun.spct)
## w.length s.irrad
## 1 297 0.0001533
## 2
        298 0.0003670
## 3
         299 0.0007845
## 4
         300 0.0012646
## 5
       301 0.0026237
## 6
      302 0.0039226
tail(trimmed.sun.spct)
      w.length s.irrad
##
## 499
         795 0.4147
## 500
          796 0.4081
## 501
           797 0.4141
## 502
           798 0.4236
## 503
           799 0.4186
## 504 800 0.4069
```

This function returns a new data.frame and uses always the same variable names for the columns.

```
trimmed.both.sun.spct <-</pre>
 trim_tails(w.length, s.e.irrad, low.limit=297, high.limit=550)
head(trimmed.both.sun.spct)
## w.length s.irrad
## 1
       297 0.0001533
## 2
         298 0.0003670
## 3
        299 0.0007845
## 4
         300 0.0012646
## 5
         301 0.0026237
         302 0.0039226
## 6
tail(trimmed.both.sun.spct)
##
     w.length s.irrad
## 249
          545 0.7272
## 250
           546 0.6993
## 251
          547 0.7119
## 252
         548 0.6937
## 253
           549 0.7021
## 254
           550 0.7047
```

If we supply a different value than the default NULL for the parameter fill, the w.length values are kept, and the trimmed spectral irradiance values replaced by the value supplied.

```
trimmed.na.sun.spct <- trim_tails(w.length, s.e.irrad, low.limit=297, fill=NA)
head(trimmed.na.sun.spct)
## w.length s.irrad</pre>
```

```
## 1 293 NA

## 2 294 NA

## 3 295 NA

## 4 296 NA

## 5 297 0.0001533

## 6 298 0.0003670
```

```
trimmed.both.na.sun.spct <-</pre>
 trim_tails(w.length, s.e.irrad, low.limit=297, high.limit=400, fill=NA)
head(trimmed.both.na.sun.spct)
##
   w.length s.irrad
## 1
       293 NA
## 2
         294
                   NA
         295
## 3
                   NA
## 4
         296
                  NA
## 5
        297 0.0001533
## 6
         298 0.0003670
tail(trimmed.both.na.sun.spct)
      w.length s.irrad
## 503
          795
                 NA
## 504
           796
                   NA
## 505
           797
                   NA
## 506
           798
                   NΑ
## 507
           799
## 508
           800
                    NA
```

In addition to NA we can supply an arbitrary numeric value.

```
trimmed.zero.sun.spct <-</pre>
 trim_tails(w.length, s.e.irrad, low.limit=297, fill=0.0)
head(trimmed.zero.sun.spct)
   w.length s.irrad
## 1
      293 0.0000000
## 2
         294 0.0000000
## 3
         295 0.0000000
## 4
         296 0.0000000
## 5
         297 0.0001533
      298 0.0003670
## 6
```

```
detach(sun.data)
```

13.2 Trimming spectral objects

We can use as above low.limit, high.limit, and fill as in the examples above.

```
trim_spct(sun.spct, low.limit=297)
##
        w.length s.e.irrad s.q.irrad
##
             297 0.0001533 3.807e-10
     1:
             298 0.0003670 9.141e-10
    2:
##
##
    3:
             299 0.0007845 1.961e-09
##
    4:
             300 0.0012646 3.171e-09
##
    5:
             301 0.0026237 6.602e-09
##
             796 0.4080616 2.715e-06
## 500·
## 501:
             797 0.4141204 2.759e-06
## 502:
             798 0.4236281 2.826e-06
## 503:
             799 0.4185850 2.796e-06
## 504:
             800 0.4069055 2.721e-06
```

We can in addition do the trimming with a waveband object.

```
trim_spct(sun.spct, PAR())
##
       w.length s.e.irrad s.q.irrad
            400 0.6081 2.033e-06
##
    1:
            401
                   0.6262 2.099e-06
##
    2:
##
    3:
            402
                   0.6497 2.183e-06
##
    4:
            403
                   0.6207 2.091e-06
                   0.6370 2.151e-06
##
    5:
            404
##
                   0.4905 2.854e-06
## 297:
            696
## 298:
            697
                   0.5165 3.009e-06
## 299:
            698
                   0.5051 2.947e-06
## 300:
            699
                   0.4834 2.824e-06
## 301:
            700
                 0.4758 2.784e-06
```

14 Optimizing performance

When developing the current version of photobiology quite a lot of effort was spent in optimizing performance, 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

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.