R for Photobiology

A handbook

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Preface

This is just a very early draft of a handbook that will accompany the release of the suite of R packages for photobiology (r4photobiology).

Acknowledgements

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List of abbreviations and symbols

For quantities and units used in photobiology we follow, as much as possible, the recommendations of the Commission Internationale de l'Éclairage as described by (Sliney 2007).

Symbol	Definition
α	(%).
Δe	water vapour pressure difference (Pa).
ϵ	emittance ($\mathrm{W\,m^{-2}}$).
λ	wavelength (nm).
θ	solar zenith angle (degrees).
ν	frequency (Hz or $\mathrm{s^{-1}}$).
ρ	(%).
σ	Stefan-Boltzmann constant.
τ	(%).
χ	water vapour content in the air ($\mathrm{g\,m^{-3}}$).
A	(absorbance units).
ANCOVA	analysis of covariance.
ANOVA	analysis of variance.
BSWF	.
c	speed of light in a vacuum.
CCD	charge coupled device, a type of light detector.
CDOM	coloured dissolved organic matter.
CFC	chlorofluorocarbons.
c.i.	confidence interval.
CIE	Commission Internationale de l'Éclairage; or erythemal action spectrum standardized by CIE.
CTC	closed-top chamber.
DAD	diode array detector, linear light detector based on photodiodes.
DBP	dibutylphthalate.
DC	direct current.
DIBP	diisobutylphthalate.
DNA(N)	UV action spectrum for 'naked' DNA.
DNA(P)	UV action spectrum for DNA in plants.
DOM	dissolved organic matter.
DU	Dobson units.
e	water vapour partial pressure (Pa).
E	(energy) irradiance ($\mathrm{W\,m^{-2}}$).
$E(\lambda)$	spectral (energy) irradiance ($\mathrm{W\,m^{-2}\,nm^{-1}}$).

E_0	fluence rate, also called scalar irradiance ($\mathrm{W\,m^{-2}}$).
ESR	early stage researcher.
FACE	free air carbon-dioxide enhancement.
FEL	a certain type of 1000 W incandescent lamp.
FLAV	UV action spectrum for accumulation of flavonoids.
FWHM	full-width half-maximum.
GAW	Global Atmosphere Watch.
GEN	generalized plant action spectrum, also abreviated as GPAS (Caldwell 1971).
GEN(G)	mathematical formulation of GEN by (Green et al. 1974) .
GEN(T)	mathematical formulation of GEN by (Thimijan et al. 1978).
h	Planck's constant.
h'	Planck's constant per mole of photons.
H	exposure, frequently called dose by biologists ($\mathrm{kJ\,m^{-2}\,d^{-1}}$).
H^{BE}	biologically effective (energy) exposure ($\mathrm{kJ\,m^{-2}\,d^{-1}}$).
$H_{\mathrm{p}}^{\mathrm{BE}}$	biologically effective photon exposure ($\mathrm{mol\,m^{-2}\,d^{-1}}$).
HPS	high pressure sodium, a type of discharge lamp.
HSD	honestly signifcant difference.
k_{B}	Boltzmann constant.
L	radiance ($\mathrm{W\,sr^{-1}\,m^{-2}}$).
LAI	leaf area index, the ratio of projected leaf area to the ground area.
LED	light emitting diode.
LME	linear mixed effects (type of statistical model).
LSD	least significant difference.
n	number of replicates (number of experimental units per treatment).
N	total number of experimental units in an experiment.
N_{A}	Avogadro constant (also called Avogadro's number).
NIST	National Institute of Standards and Technology (U.S.A.).
NLME	non-linear mixed effects (statistical model).
OTC	open-top chamber.
PAR	, 400–700 nm.
	measured as energy or photon irradiance.
PC	polycarbonate, a plastic.
PG	UV action spectrum for plant growth.
PHIN	UV action spectrum for photoinhibition of isolated chloroplasts.
PID	(control algorithm).
PMMA	polymethylmethacrylate.
PPFD	, another name for
	PAR photon irradiance (Q_{PAR}).
PTFE	polytetrafluoroethylene.
PVC	polyvinylchloride.
q	energy in one photon ('energy of light').
q'	energy in one mole of photons.
Q	photon irradiance ($\mathrm{mol\,m^{-2}\,s^{-1}}$ or $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$).
$Q(\lambda)$	spectral photon irradiance ($\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$ or $\mathrm{\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}}$).
r_0	distance from sun to earth.
RAF	(nondimensional).
RH	relative humidity (%).
s	energy effectiveness (relative units).

$s(\lambda)$	spectral energy effectiveness (relative units).
s^{p}	quantum effectiveness (relative units).
$s^{\mathrm{p}}(\lambda)$	spectral quantum effectiveness (relative units).
s.d.	standard deviation.
SDK	software development kit.
s.e.	standard error of the mean.
SR	spectroradiometer.
t	time.
T	temperature.
TUV	tropospheric UV.
U	electric potential difference or voltage (e.g. sensor output in V).
UV	ultraviolet radiation (λ = 100–400 nm).
UV-A	ultraviolet-A radiation (λ = 315–400 nm).
UV-B	ultraviolet-B radiation (λ = 280–315 nm).
UV-C	ultraviolet-C radiation (λ = 100–280 nm).
$\mathrm{UV}^{\mathrm{BE}}$	biologically effective UV radiation.
UTC	coordinated universal time, replaces GMT in technical use.
VIS	radiation visible to the human eye ($\approx$ 400–700 nm).
WMO	World Meteorological Organization.
VPD	water vapour pressure deficit (Pa).
WOUDC	World Ozone and Ultraviolet Radiation Data Centre.

Part I

Theory behind calculations

Part II

Tools used for calculations

CHAPTER 1

Photobiology R packages

Abstract

In this chapter we describe the suite of R packages for photobiological calculations 'r4photobiology', and explain how to install them.

1.1 Expected use and users

The aim of the suite is to both provide a framework for teaching VIS and UV radiation physics and photobiology through a set of functions and data examples. Furthermore, we expect these functions and data to be useful for active researchers during design of experiments, data analysis and data validation. In particular we hope the large set of example data will make it easy to carry out sanity checks of newly acquired and/or published data.

Given the expected audience of both students and biologists, rather than data analysts, or experienced programmers, we have aimed at designing a consistent and easy to understand paradigm for the analysis of spectral data. The design is based on our own user experience, and on feedback from our students and 'early adopters'.

1.2 The design of the framework

The design of the 'high level' interface is based on the idea of achieving simplicity of use by hiding the computational difficulties and exposing objects, functions and operators that map directly to physical concepts. Computations and plotting of spectral data centers on two types of objects: *spectra* and *wavebands* (Figure 1.1). Al spectra have in common that observations are referenced to a wavelength value. However, there are different types spectral objects, e.g. for light sources and responses to light. Waveband objects include much more

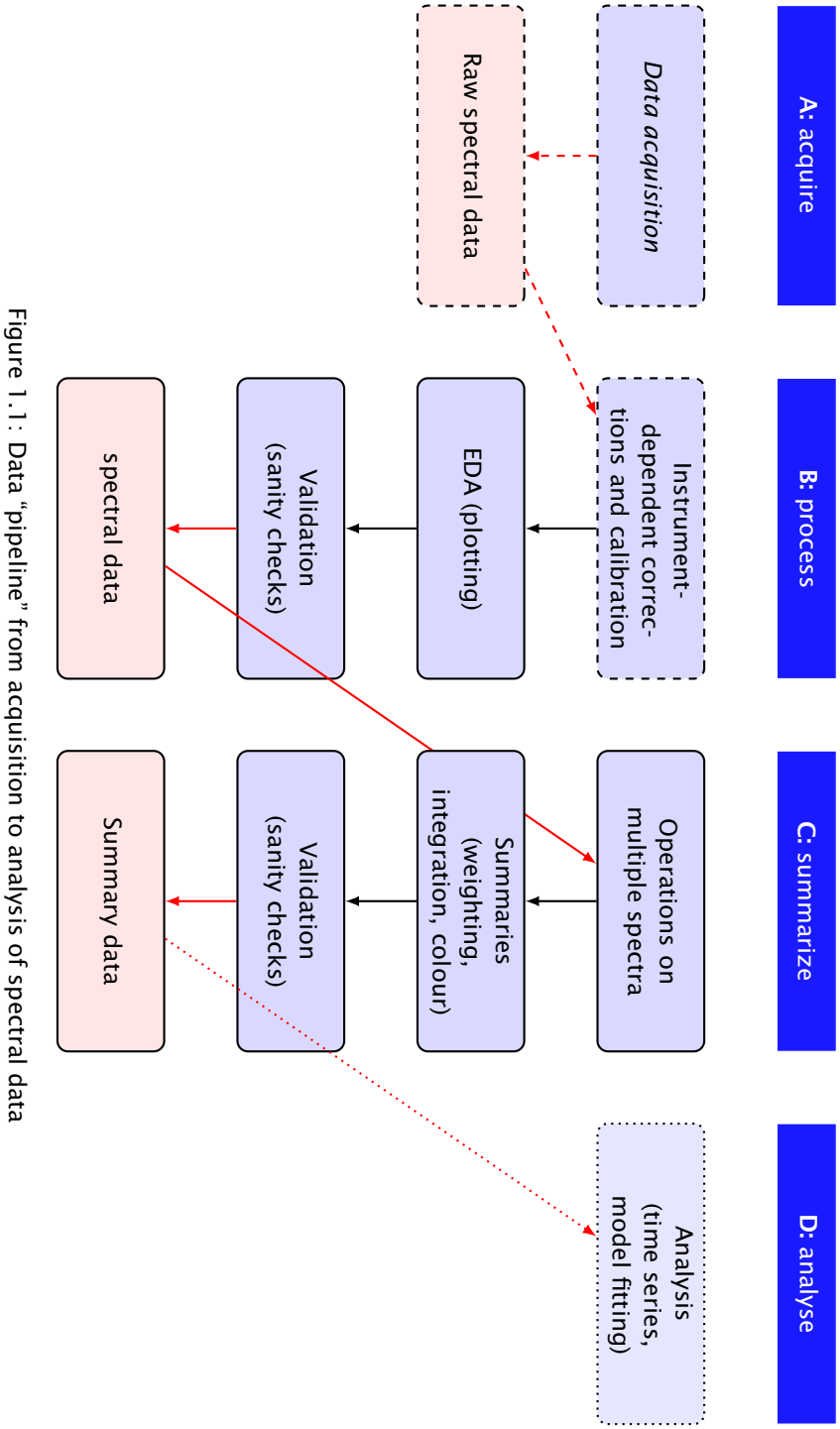

Figure 1.1: Data "pipeline" from acquisition to analysis of spectral data

textbox 1.1: Elements of the framework used by all packages in the suite.

`_spct` Spectral objects are containers for different types of spectral data, data which is referenced to wavelength. These data normally originate in measurements or simulation with models.

`_multi_spct` Containers for spectral objects are used to store related spectral objects, such as time series of spectral objects or spectral images.

`wavebands` Waveband objects are containers of 'instructions' for the quantification of spectral data. In addition to the everyday definition as a range of wavelengths, we include the spectral weighting functions used in the calculation of what are frequently called weighted or effective exposures and doses.

summary functions Different summary functions return different quantities through integration over wavelengths and take as arguments spectra and wavebands.

maths operators and functions Are used to combine and/or transform spectral data, and in some cases to apply weights defined by wavebands.

than information about a range of wavelengths, they can also include information about a transformation of the spectral data, like a biological spectral weighting function (BSWF). In addition to functions for calculating summary quantities like irradiance from spectral irradiance, the packages define operators for spectra and wavebands. The use of operators simplifies the syntax and makes the interface easier to use.

A consistent naming scheme as well as consistency in the order of function arguments across the suite.... Data objects are *tidy* as defined by in (**Wickham2013**), in other words data on a row always corresponds to a single observation event, although such an observation can consist in more than one measured or derived quantity. Data from different observations are stored in different objects, or if in the same object they are *keyed* using and index variable.

The same summary methods, are available for `_spct` and `_multi_spct`, in the first case returning a vector, and in the second case, a `data.frame` object.

Package `photobiology` can be thought as a framework defining a way of storing spectral data plus 'pieces' from which specific summaries can be constructed. Extensibility and reuse is at the core of the design. This is achieved by using the weakest possible assumptions or expectations about data properties and avoiding as much as possible the hard-coding of any constants or size limits. This, of course, has a cost in possibly slower execution speed.

Within these constraints an effort has been made to remove performance bottleneck by means of C++ code and passing data objects by reference when possible.

```
e_irrad(sun.spct * polyester.new.spct, CIE())
```

Is all what is needed to obtain the CIE98-weigthed energy irradiance simulating the effect of a polyester filter on the example solar spectrum, which of course, can be substituted by other spectral irradiance and filter data.

When we say that we hide the computational difficulties what we mean, is that in the example above, the data for the two spectra do not need to be available at the same wavelengths values, and the BSWF is defined as a function. Interpolation of the spectral data and calculation of spectral weighting factors takes place automatically and invisibly. All functions and operators function without error with spectra with varying (even arbitrarily and randomly varying) wavelength steps. Integration is always used rather than summation for summarizing the spectral data.

There is a lower layer of functions, used internally, but also exported, which allow improved performance at the expense of more complex scripts and commands. This user interface is not meant for the casual user, but for the user who has to analyse thousands of spectra and uses scripts for this. For such users performance is the main concern rather than easy of use and easy to remember syntax. Also these functions handle any wavelength mismatch by interpolation before applying operations or functions.

The suite also includes data for the users to try options and ideas, and helper functions for plotting spectra using other R packages available from CRAN, in particular `ggplot2`. There are some packages, not part of the suite itself, for data acquisition from Ocean Optics spectrometers, and application of special calibration and correction procedures to those data. A future package will provide an interface to the TUV model to allow easy simulation of the solar spectrum.

1.3 The suite

The suite consists in several packages. The main package is `photobiology` which contains all the generally useful functions, including many used in the other, more specialized, packages (Table 1.1).

Spectral irradiance objects (class `source_spct`) and spectral response/action objects (class `response_spct`) can be constructed using energy- or photon-based data, but this does not affect their behaviour. The same flexibility applies to spectral transmittance vs. spectral absorbance for classes `filter_spct`, `reflector_spct` and `object_spct`.

Although by default low-level functions expect spectral data on energy units, this is just a default that can be changed by setting the parameter `unit.in = "photon"`. Across all data sets and functions wavelength vectors have name `w.length`, spectral (energy) irradiance `s.e.irrad`, photon spectral irradiance `s.q.irrad`[1], absorbance ($\log_{10}$-based) `A`, transmittance (fraction of one)

[1] `q` derives from 'quantum'.

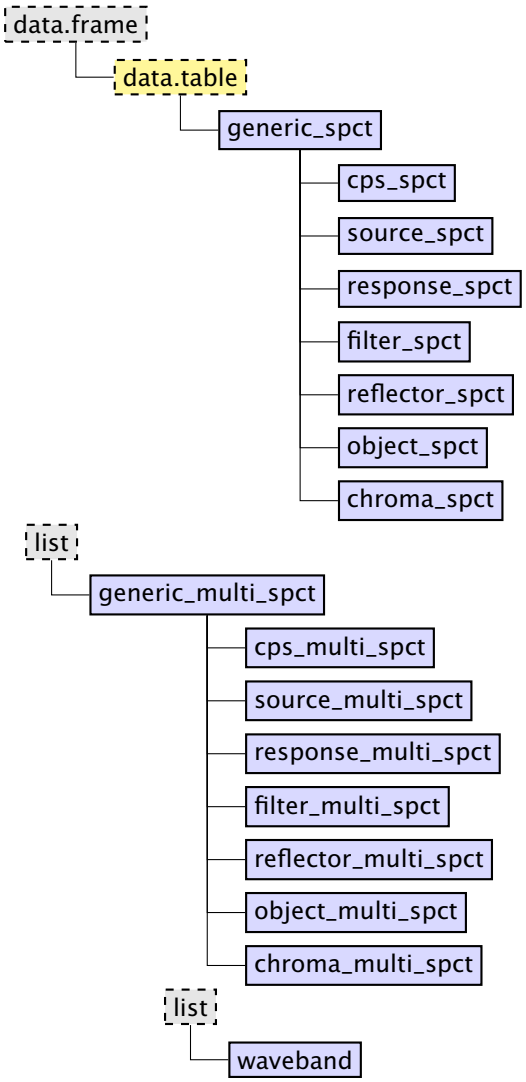

Figure 1.2: Object classes used in the packages. Objects of `_spct` classes are used to store spectra, in most cases a single spectrum. Objects of `_multi_spct` classes can be used to store *collections* of `_spct` objects, in most cases all belonging to the same class. Objects of class `waveband` contain information used for quantification: boundaries of a wavelength range and, optionally, spectral weighting functions. Gray-filled boxes represent classes defined in base R, yellow-filled boxes represent classes defined by contributed packages available through , and blue-filled boxes represent classes defined in package photobiology.

Table 1.1: Packages in the r4photobiology suite. Packages not yet released are highlighted with a red bullet •, and those at 'beta' stage with a yellow bullet •, those relatively stable with a green bullet •.

	Package	Type	Contents
•	photobiologyAll	dummy	loads other packages of the suite
•	photobiology	funs + classes	basic functions, class definitions, class methods and example data
•	photobiologyInOut	functions	data import/export functions
•	photobiologyWavebands	definitions	quantification of radiation
•	photobiologygg	functions	extensions to package `ggplot2`
•	photobiologySun	data	spectral data for solar radiation
•	photobiologyLamps	data	spectral data for lamps
•	photobiologyLEDs	data	spectral data for LEDs
•	photobiologyFilters	data	transmittance data for filters
•	photobiologySensors	data	response data for sensors
•	photobiologyReflectors	data	reflectance data for materials
•	photobiologyPlants	funs + data	photobiology of plants
•	rOmniDriver	functions	Ocean Optics spectrometers
•	MayaCalc	functions	UV and VIS irradiance data processing for Maya2000 Pro
•	rTUV	funs + data	TUV model interface

`Tfr`, transmittance (%) `Tpc`, reflectance (fraction of one) `Rfr`, reflectance (%) `Rpc`, and absorptance (fraction of one) `Afr`.

Wavelengths should always be in naanometres (nm), and when conversion between energy and photon based units takes place no scaling factor is used (an input in $\mathrm{W\,m^{-2}\,nm^{-1}}$ yields an output in $\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$ rather than $\mathrm{\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}}$).

The suite is still under active development. Even those packages marked as 'stable' are likely to acquire new functionality. By stability, we mean that we hope to be able to make most changes backwards compatible, in other words, we hope they will not break existing user code.

1.4 The r4photobiology repository

I have created a repository for the packages. This repository follows the CRAN folder structure, so package installation can be done using normal R commands. This means that dependencies are installed automatically and that automatic updates are possible. The build most suitable for the current system and R version is also picked automatically if available. It is normally recommended that you do installs and updates on a clean R session (just after starting R or RStudio). For easy installation and updates of packages, the r4photobiology repository can be added to the list of repositories that R knows about.

Whether you use RStudio or not it is possible to add the r4photobiology repository to the current session as follows, which will give you a menu of additional repositories to activate:

```
setRepositories(
  graphics = getOption("menu.graphics"),
  ind = NULL,
  addURLs = c(r4photobiology = "http://www.r4photobiology.info/R"))
```

If you know the indexes in the menu you can use this code, where '1' and '6' are the entries in the menu in the command above.

```
setRepositories(
  graphics = getOption("menu.graphics"),
  ind = c(1, 6),
  addURLs = c(r4photobiology = "http://www.r4photobiology.info/R"))
```

Be careful not to issue this command more than once per R session, otherwise the list of repositories gets corrupted by having two repositories with the same name.

Easiest is to create a text file and name it '`.Rprofile`', unless it already exists. The commands above (and any others you would like to run at R start up) should be included, but with the addition that the package names for the functions need to be prepended. So previous example becomes:

```
utils::setRepositories(
  graphics = getOption("menu.graphics"),
  ind = c(1, 6),
  addURLs = c(r4photobiology = "http://www.r4photobiology.info/R"))
```

The `.Rprofile` file located in the current folder is sourced at R start up. It is also possible to have such a file affecting all of the user's R sessions, but its location is operating system dependent, it is in most cases what the OS considers the current user's *HOME* directory or folder (e.g. 'My Documents' in recent versions of MS-Windows). If you are using RStudio, after setting up this file, installation and updating of the packages in the suite can take place exactly as for any other package archived at CRAN.

The commands and examples below can be used at the R prompt and in scripts whether RStudio is used or not.

After adding the repository to the session, it will appear in the menu when executing this command:

```
setRepositories()
```

and can be enabled and disabled.

In RStudio, after adding the r4photobiology repository as shown above, the photobiology packages can be installed and uninstalled through the normal RStudio menus and dialogues, and will listed after typing the first few characters of their names. For example when you type 'photob' in the packages field, all the packages with names starting with 'photob' will be listed.

They can be also installed at the R command prompt with the following command:

```
install.packages(c("photobiologyAll", "photobiologygg"))
```

and updated with:

```
update.packages()
```

The added repository will persist only during the current R session. Adding it permanently requires editing the R configuration file, as discussed above. Take into consideration that `.Rprofile` is read by R itself, and will take effect whether you use RStudio or not. It is possible to have an user-account wide .Rprofile file, and a different one on those folders needing different settings. Many other R options can also be modified by means of commands in the .Rprofile file.

Part III

Cookbook of calculations

Part IV

Data acquisition and modelling

Part V

Catalogue of example data

Part VI

Optimizing computation speed

Authors' note: *Chapter not included as example code is giving errors at the moment.*

CHAPTER 2

Further reading

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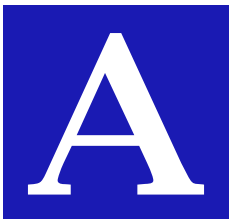
Part VII

Appendix

APPENDIX



Build information

```
Sys.info()
```

```
##                       sysname
##                     "Windows"
##                       release
##                       "7 x64"
##                       version
## "build 7601, Service Pack 1"
##                      nodename
##                       "MUSTI"
##                       machine
##                      "x86-64"
##                         login
##                      "aphalo"
##                          user
##                      "aphalo"
##                 effective_user
##                      "aphalo"
```

```
sessionInfo()
```

```
## R version 3.2.1 (2015-06-18)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
## Running under: Windows 7 x64 (build 7601) Service Pack 1
##
## locale:
## [1] LC_COLLATE=English_United Kingdom.1252
## [2] LC_CTYPE=English_United Kingdom.1252
## [3] LC_MONETARY=English_United Kingdom.1252
## [4] LC_NUMERIC=C
## [5] LC_TIME=English_United Kingdom.1252
##
## attached base packages:
## [1] tools     stats     graphics  grDevices
```

```
## [5] utils     datasets  base
##
## other attached packages:
## [1] stringr_1.0.0 knitr_1.10.5
##
## loaded via a namespace (and not attached):
## [1] magrittr_1.5  formatR_1.2   stringi_0.5-5
## [4] highr_0.5     evaluate_0.7
```