R for Photobiology

A handbook

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Preface

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

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 Sliney2007.

| Symbol | Definition |
|--------------|---|
| α | (%). |
| Δe | water vapour pressure difference (Pa). |
| ϵ | emittance ($W m^{-2}$). |
| λ | wavelength (nm). |
| θ | solar zenith angle (degrees). |
| ν | frequency (Hz or s^{-1}). |
| ρ | (%). |
| σ | Stefan-Boltzmann constant. |
| τ | (%). |
| χ | water vapour content in the air ($g m^{-3}$). |
| A | (absorbance units). |
| ANCOVA | analysis of covariance. |
| ANOVA | analysis of variance. |
| BSWF | |
| С | 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 (Wm^{-2}). |
| $E(\lambda)$ | spectral (energy) irradiance ($W m^{-2} nm^{-1}$). |

 E_0 fluence rate, also called scalar irradiance (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 Caldwell1971.

GEN(G) mathematical formulation of GEN by Green1974.
GEN(T) mathematical formulation of GEN by Thimijan1978.

h Planck's constant.

h' Planck's constant per mole of photons.

H exposure, frequently called dose by biologists (kJ m⁻² d⁻¹).

 H^{BE} biologically effective (energy) exposure (kJ m⁻² d⁻¹). $H^{\mathrm{BE}}_{\mathrm{p}}$ biologically effective photon exposure (mol m⁻² d⁻¹). HPS high pressure sodium, a type of discharge lamp.

HSD honestly significant difference.

 $k_{\rm B}$ Boltzmann constant. L radiance (Wsr⁻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. $N_{\rm A}$ 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 ($mol m^{-2} s^{-1}$ or $\mu mol m^{-2} s^{-1}$).

 $Q(\lambda)$ spectral photon irradiance (mol m⁻² s⁻¹ nm⁻¹ or μ 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).

 $s^{p}(\lambda)$ 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).

 $\begin{array}{ll} UV & ultraviolet\ radiation\ (\lambda=100\text{-}400\ nm). \\ UV\text{-}A & ultraviolet\text{-}A\ radiation\ (\lambda=315\text{-}400\ nm). \\ UV\text{-}B & ultraviolet\text{-}B\ radiation\ (\lambda=280\text{-}315\ nm). \\ UV\text{-}C & ultraviolet\text{-}C\ radiation\ (\lambda=100\text{-}280\ nm). \end{array}$

UV^{BE} biologically effective UV radiation.

UTC coordinated universal time, replaces GMT in technical use.

VIS radiation visible to the human eye ($\approx 400\text{--}700 \text{ nm}$).

WMO World Meteorological Organization. VPD water vapour pressure deficit (Pa).

WOUDC World Ozone and Ultraviolet Radiation Data Centre.

Part I Getting ready

CHAPTER

Introduction

Abstract

In this chapter we explain the physical basis of optics and photochemisatry.

1.1 Radiation and molecules

CHAPTER

Optics

Abstract

In this chapter we explain how to .

2.1 Task:



Photochemistry

Abstract

In this chapter we explain how to .

3.1 Task:



Software

Abstract

In this chapter we explain how to .

4.1 Task:



Photobiology R pacakges

Abstract

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

5.1 The suite

The suite consists in several packages. The main package is photobiology which contains all the generaly useful functions, including many used in the other, more especialized, packages (Table 5.1).

5.2 photoCRAN repository

I have created a small repository for the packages. This repository follows the CRAN folder structure, so now package installation can be done using just the 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 photoCRAN repo can be added to the list of repos that R knows about.

Whether you use RStudio or not it is possible to add the photoCRAN repo to the current session as follows:

Table 5.1: Packages in the r4photobiology suite. Packages not yet released are higlighted with a red bullet, and those at 'beta' stage with a yellow bullet, those relatively stable with a green bullet.

| Package | Type | Contents |
|--|--|---|
| photobiology | functions | basic functions and example data |
| photobiologyVISphotobiologyUV | definitions definitions | quantification of VIS radiation quantification of UV radiation |
| photobiologySun photobiologyLamps photobiologyLEDs photobiologyFilters photobiologySensors | data data data data data | spectral data for solar radiation spectral data for lamps spectral data for LEDs transmittance data for filters response data for broadband sensors |
| photobiologyPhyphotobiologyCryphotobiologyPhotphotobiologyUVR8 | funs + data funs + data funs + data funs + data | phytochromes cryptochromes phototropins phototropins |
| photobiologygg | funtions | extensions to package ggplot2 |
| rTUVrOmniDriver | funs + data functions | TUV model interface control of Ocean Optics spectrometers |

which will give you a menu of additional repos to activate.

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.

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

After adding the repo 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 photoCRAN repo as shown above, the photobiology packages can be installed and uninstalled through the normal RStudio menues and dialogues. 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 with:

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

and updated with:

```
update.packages()
```

The added repo will persist only during the current R session. Adding it permanently requires editing the R configuration file.

5.3 How to install the pakages

The examples given in this page assume that photoCRAN is not in the list of repos known to the current R session. See the section 5.2 on the photoCRAN repo for an alternative to the approach given here.

To install the latest version of one package (photobiology used as example) you just need to indicate the repository. However this simple command will only install the dependencies bewteen the different photobiology packages.

To update what is already installed, this command is enough (even if the packages have been installed manually before):

```
update.packages(repos = "http://www.mv.helsinki.fi/aphalo/R")
```

The best way to install the packages is to specify both my repo and a normal CRAN repo, then all dependencies will be automatically installed. The new package photobiolgyAll just loads and imports all the packages in the suite, except for photobiolygg. Because of this dependency all the packages are installed unless already installed.

This example also shows how one can use an array of package names (in this example all my currently available photobiology packages) in the call to the function install.packages, this is useful if you want to install only a subset of the files, or if you want to make sure that any older install of the packages is overwritten:

The commands above install all my packages and all their dependencies from CRAN if needed. The following command will update all the packages

currently installed (if new versions are available) and install any new dependencies.

The instructions above should work under Windows as long as you have a supported version of R (3.0.0 or later) because I have built suitable binaries, under other OS you may need to add type="source" unless this is already the default. We will try to build OS X binaries for Mac so that installation is easier. Meanwhile if installation fails try adding type="source" to the commands given above. For example the first one would become:

When using type=source you may need to install some dependencies like the splus2R package beforehand from CRAN if building it from sources fails.

Part II

Cookbook

Unweighted irradiance

Abstract

In this chapter we explain how to calculate unweighted energy and photon irradiances from spectral irradiance.

6.1 Task: (energy) irradiance from spectral irradiance

The task to be completed is to calculate the (energy) irradiance (E) in W m⁻² from spectral (energy) irradiance ($Q(\lambda)$) in W m⁻² nm⁻¹ and the corresponding wavelengths (λ) in nm.

$$Q_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda) \, d\lambda$$
 (6.1)

Let's assume that we want to calculate photosynthetically active radiation (PAR) energy irradiance, for which the most accepted limits are $\lambda_1 = 400$ nm and $\lambda_1 = 700$ nm. In this example we will use example data for sunlight to calculate $E_{400\,\mathrm{nm}<\lambda<700\,\mathrm{nm}}$:

Function PAR() is predefined in package photobiologyVIS as a convenience function, so the code above can be replaced by:

```
with(sun.data, energy_irradiance(w.length, s.e.irrad, PAR()))
## PAR
## 196.7
```

If no waveband is supplied as argument, then the whole range of wavelengths in the spectral data is used for the integration, and the 'name' attribute is generated accordingly:

```
with(sun.data, energy_irradiance(w.length, s.e.irrad))
## range.293.800
## 268.9
```

If a waveband that does not fully overlap with the data is supplied as argument, then spectral irradiance for wavelengths outside the range is assumed to be zero:

If a waveband that does not overlap with the data is supplied as argument, then spectral irradiance for wavelengths outside the range is assumed to be zero:

6.2 Task: photon irradiance from spectral irradiance

The task to be completed is to calculate the photon irradiance (Q) in $\mod m^{-2}$ s⁻¹ from spectral (energy) irradiance $(E(\lambda))$ in Wm^{-2} nm⁻¹ and the corresponding wavelengths (λ) in nm.

The energy of a quantum of radiation in a vacuum, q, depends on the wavelength, λ , or frequency¹, ν ,

$$q = h \cdot \nu = h \cdot \frac{c}{\lambda} \tag{6.2}$$

with the Planck constant $h = 6.626 \times 10^{-34}$ Js and speed of light in vacuum $c = 2.998 \times 10^8$ m s⁻¹. When dealing with numbers of photons, the equation (6.2) can be extended by using Avogadro's number $N_{\rm A} = 6.022 \times 10^{23}$ mol⁻¹. Thus, the energy of one mole of photons, q', is

$$q' = h' \cdot \nu = h' \cdot \frac{c}{\lambda} \tag{6.3}$$

with $h' = h \cdot N_A = 3.990 \times 10^{-10} \text{ Js mol}^{-1}$. Example 1: red light at 600 nm has about 200 kJ mol⁻¹, therefore, 1 μ mol photons has 0.2 J. Example 2: UV-B

 $^{^1}$ Wavelength and frequency are related to each other by the speed of light, according to $\nu=c/\lambda$ where c is speed of light in vacuum. Consequently there are two equivalent formulations for equation 6.2.

radiation at 300 nm has about $400~\rm kJ\,mol^{-1}$, therefore, $1~\mu\rm mol$ photons has 0.4 J. Equations 6.2 and 6.3 are valid for all kinds of electromagnetic waves. Combining equations 6.1 and 6.3 we obtain:

$$Q_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda) \, \frac{h' \cdot c}{\lambda} \mathrm{d} \, \lambda \tag{6.4}$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) photon irradiance. In this example we will use example data for sunlight.

If we want to have Q_{PAR} (PPFD) expressed in the usual units of μ mol m⁻² s⁻¹, we need to multiply the result above by 10^6 :

PAR() is predefined in package photobiologyVIS as a convenience function, see section 6.1 for an example with arbitrary values for λ_1 and λ_2 .

6.3 Task: calculate energy and photon irradiances from spectral photon irradiance

In the case of the calculation of energy irradiance from spectral photon irradiance the calculation is:

$$I_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} Q_{\lambda} \, \frac{\lambda}{h' \cdot c} \mathrm{d} \, \lambda \tag{6.5}$$

And the code²:

```
with(sun.data, energy_irradiance(w.length, s.q.irrad, PAR()),
     unit.in = "photon")

## PAR
## 0.0008938
```

The calculation of photon irradiance from spectral photon irradiance, is a simple integration, analogous to that in equation 6.1, and the code is:

```
with(sun.data, photon_irradiance(w.length, s.q.irrad, PAR()),
    unit.in = "photon")

## PAR
## 4.158e-09
```

²The dataframe sun.data contains both spectral energy irradiance vales in 'column' s.e.irrad and spectral photon irradiance in 'column' s.q.irrad

6.4 Task: irradiances for more than one waveband

It is possible to calculate the irradiances for several wavebands with a single function call by supplying a list of wavebands as argument:

```
with(sun.data, photon_irradiance(w.length, s.e.irrad, list(Red(),
   Green(), Blue()))) * 1e+06
    Red.ISO Green.ISO Blue.ISO
      452.2
##
               220.2
                          149.0
Q.RGB <- with(sun.data, photon_irradiance(w.length, s.e.irrad,
list(Red(), Green(), Blue()))) * 1e+06
signif(Q.RGB, 3)
##
    Red.ISO Green.ISO Blue.ISO
                  220
##
        452
Q.RGB[1]
## Red.ISO
##
   452.2
Q.RGB["Green.ISO"]
## Green.ISO
## 220.2
```

A named list can be used to override the use as names for the output of the waveband names:

Even when using a single waveband:

6.5 Task: use simple wavebands

Please, consult the packages' documentation for a list of predefined functions for creating wavebands. Here we will present just a few examples of their use. We usually associate wavebands with colours, however, in many cases there are different definitions in use. For this reason, the functions provided accept an argument that can be used to select the definition to use. In general, the default, is to use the ISO standard whenever it is applicable. The case of the various definitions in use for the UV-B waveband are described on page 21

We can use a predefined function to create a new waveband object, which as any other R object can be assigned to a variable:

```
uvb <- UVB()
uvb

## UVB.ISO
## low (nm) 280
## high (nm) 315</pre>
```

As seen above, there is a specialized print function for wavebands. Functions available are min, max, range, center_wl, labels, and color.

```
red <- Red()
red
## Red.ISO
## low (nm) 610
## high (nm) 760
min(red)
## [1] 610
max(red)
## [1] 760
range(red)
## [1] 610 760
midpoint(red)
## [1] 685
labels(red)
## $label
## [1] "Red.ISO"
color(red)
## Red.ISO CMF Red.ISO CC
## "#900000" "#FF0000"
```

Here we demonstrate the use of an argument to choose a certain definition:

```
UVB()
## UVB.ISO
## low (nm) 280
## high (nm) 315

UVB("ISO")
## UVB.ISO
## low (nm) 280
## high (nm) 315
```

```
UVB("CIE")

## UVB.CIE

## low (nm) 280

## high (nm) 315

UVB("medical")

## UVB.medical

## low (nm) 290

## high (nm) 320

UVB("none")

## UVB.none

## low (nm) 280

## high (nm) 320
```

Here we demonstrate the importance of complying with standards, and how much the photon irradiance calculated can depend on the definition used.

6.6 Task: define simple wavebands

Here we briefly introduce new_waveband, and only in chapter ?? we describe its use in full detail, including the use of spectral weighting functions (SWFs).

Defining a new waveband based on extreme wavelengths expressed in nm.

6.7 Task: photon ratios

In photobiology sometimes we are interested in calculation the photon ratio between two wavebands. It makes more sense to calculate such ratios if both numerator and denominator wavebands have the same 'width' or if the numerator waveband is fully nested in the denominator waveband. However, frequently used ratios like the UV-B to PAR photon ratio do not comply with this. For this reason, our functions do not enforce any such restrictions.

For example a ratio frequently used in plant photobiology is the read to farred photon ratio (R:FR photon ratio or ζ). If we follow the wavelength ranges in the definition given by **Morgan1981a** using photon irradiance³:

$$\zeta = \frac{Q_{655\text{nm}} < \lambda < 665\text{nm}}{Q_{725\text{nm}} < \lambda < 735\text{nm}}$$
(6.6)

To calculate this for our example sunlight spectrum we can use the following code:

or using the predefined convenience function R_FR_ratio:

Using defaults for waveband definitions:

```
with(sun.data,
          energy_ratio(w.length, s.e.irrad, UVB(), PAR()))
## [1] 0.00299
```

 $^{^3}$ In the original text photon fluence rate is used but it not clear whether photon irradiance was meant instead.

6.8 Task: energy ratios

An energy ratio, equivalent to ζ can be calculated as follows:

```
with(sun.data,
          energy_ratio(w.length, s.e.irrad, Red("Smith"), Far_red("Smith")))
## [1] 1.384
```

For this infrequently used ratio, no pre-defined function is provided.

6.9 Task: calculate average number of photons per unit energy

When comparing photo-chemical and photo-biological responses under different light sources it is of interest to calculate the photons per energy in $\mathrm{mol}\,\mathrm{W}^{-1}$. In this case only one waveband definition is used to calculate the quotient:

$$\bar{q'} = \frac{Q_{\lambda_1 < \lambda < \lambda_2}}{E_{\lambda_1 < \lambda < \lambda_2}} \tag{6.7}$$

For obtaining the same quotient in μ mol W⁻¹ we just need to multiply by 10^6 . We can use such a multiplier to convert E [W m⁻²] into Q [μ mol m⁻² s⁻¹], or as a divisor to convert Q [μ mol m⁻² s⁻¹] into E [W m⁻²], for a given light source and waveband:

6.10 Task: calculate the contribution of different regions of a spectrum to energy irradiance

It can be of interest to split the total (energy) irradiance into adjacent regions delimited by arbitrary wavelengths. We can use the function split_energy_irradiance to obtain to energy of each of the regions delimited by the values in nm supplied in a numeric vector:

Here we demonstrate that the sum of the four 'split' irradiances add to the total for the range of wavelengths covered:

It also possible to obtain the 'split' as a vector of fractions adding up to one,

or as percentages:

A vector of two wavelengths is valid input, although not very useful for percentages:

Although for scale="absolute", the default, it can be used as a quick way of calculating an irradiance for a range of wavelengths without having to define a waveband:

6.11 Task: calculate the contribution of different regions of a spectrum to photon irradiance

The function split_photon_irradiance takes the same arguments as the equivalent function for photon irradiance, consequently only one code example is provided here (see section 6.10 for more details):



Weighted and effective irradiance

Abstract

In this chapter we explain how to .



Colour

Abstract

In this chapter we explain how to .



Photoreceptors

Abstract

In this chapter we explain how to .



Radiation sources

Abstract

In this chapter we explain how to .



Filters

Abstract

In this chapter we explain how to .

CHAPTER 1

Plotting spectra

Abstract

In this chapter we explain how to .

CHAPTER 1

Calibration

Abstract

In this chapter we explain how to .

CHAPTER

THAPTER

Simulation

Abstract

In this chapter we explain how to .



Measurement

Abstract

In this chapter we explain how to .

Optimizing performance

Abstract

In this chapter we explain how to .