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

Preliminaries

Part II

Cookbook of calculations

CHAPTER 1

Simple summaries and spectral features

Abstract

In this chapter we explain how to obtain different summaries common to all types of spectral data. In addition we describe how to extract spectral features from spectral data.

1.1 Packages used in this chapter

For executing the examples listed in this chapter you need first to load the following packages from the library:

```
library(photobiology)

## Loading required package:  data.table

library(photobiologygg)

## Loading required package:  photobiologyWavebands
## Loading required package:  proto
## Loading required package:  ggplot2
## Loading required package:  methods
## Loading required package:  scales

library(photobiologyLamps)
```

1.2 Task: Summaries related to wavelength

Functions `max`, `min`, `range`, `midpoint` when used with an object of class `generic_spct` (or a derived class) return the result of applying these functions to the `w.length` component of these objects, returning always values expressed in nanometres as long as the objects have been correctly created.

```
range(sun.spct)

## [1] 293 800

midpoint(sun.spct)

## [1] 546.5

max(sun.spct)

## [1] 800

min(sun.spct)

## [1] 293
```

Functions `spread` are `stepsize` are generics defined in package photobiology. `spread` returns maximum less minimum wavelengths values in nanometres, while `stepsize` returns a numeric vector of length two with the maximum and the minimum wavelength step between observations, also in nanometers.

```
spread(sun.spct)

## [1] 507

stepsize(sun.spct)

## [1] 1 1
```

In the case of the `summary` method, specializations for `source_spct` and ... are provided. But for other spectral objects, the `summary` method for `data.table` is called. For the `summary` specializations defined, the corresponding `print` method specializations are also defined.

```
summary(sun.spct)

## 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
```

1.3 Task: Find peaks and valleys

1.3.1 Obtaining the location of peaks as an index into the spectral data

Function `find_peaks`, takes as argument a `numeric` vector, and returns a logical vector of the same length, with TRUE for local maxima and FALSE for all other observations. Infinite values are discarded.

```r
find_peaks(sun.spct$s.e.irrad)

##   [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##   [8] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [15] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [22] FALSE  TRUE FALSE  TRUE FALSE FALSE FALSE
##  [29]  TRUE FALSE FALSE FALSE FALSE FALSE  TRUE
##  [36] FALSE FALSE  TRUE FALSE  TRUE FALSE FALSE
##  [43]  TRUE FALSE FALSE FALSE FALSE  TRUE FALSE
##  [50] FALSE  TRUE FALSE  TRUE FALSE  TRUE FALSE
##  [57] FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE
##  [64] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
##  [71] FALSE  TRUE FALSE  TRUE FALSE FALSE FALSE
##  [78]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
##  [85] FALSE  TRUE FALSE FALSE  TRUE FALSE FALSE
##  [92] FALSE  TRUE FALSE  TRUE FALSE FALSE FALSE
##  [99]  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE
## [106] FALSE FALSE FALSE FALSE  TRUE FALSE  TRUE
## [113] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
## [120]  TRUE FALSE  TRUE FALSE  TRUE FALSE FALSE
## [127]  TRUE FALSE  TRUE FALSE FALSE FALSE FALSE
## [134]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## [141]  TRUE FALSE FALSE  TRUE FALSE FALSE FALSE
## [148] FALSE FALSE  TRUE FALSE  TRUE FALSE FALSE
## [155] FALSE  TRUE FALSE FALSE  TRUE FALSE FALSE
## [162] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
## [169]  TRUE FALSE FALSE  TRUE FALSE  TRUE FALSE
## [176]  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE
## [183]  TRUE FALSE FALSE  TRUE FALSE  TRUE FALSE
## [190]  TRUE FALSE FALSE FALSE FALSE FALSE  TRUE
## [197] FALSE  TRUE FALSE FALSE  TRUE FALSE  TRUE
## [204] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
## [211]  TRUE FALSE FALSE  TRUE FALSE FALSE  TRUE
## [218] FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE
## [225] FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE
## [232] FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE
## [239]  TRUE FALSE FALSE FALSE FALSE  TRUE FALSE
## [246]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## [253]  TRUE FALSE  TRUE FALSE FALSE  TRUE FALSE
## [260]  TRUE FALSE FALSE  TRUE FALSE FALSE  TRUE
## [267] FALSE FALSE  TRUE FALSE  TRUE FALSE  TRUE
## [274] FALSE FALSE  TRUE FALSE  TRUE FALSE FALSE
## [281]  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE
## [288] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
## [295]  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE
## [302]  TRUE FALSE FALSE  TRUE FALSE FALSE  TRUE
## [309] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
## [316]  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE
## [323]  TRUE FALSE FALSE FALSE  TRUE FALSE  TRUE
## [330] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
## [337]  TRUE FALSE FALSE FALSE  TRUE FALSE  TRUE
## [344] FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE
## [351] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [358] FALSE  TRUE FALSE  TRUE FALSE FALSE FALSE
## [365] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
## [372] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
## [379] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
## [386] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [393] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
## [400]  TRUE FALSE FALSE FALSE FALSE  TRUE FALSE
```

```
## [407] FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
## [414] FALSE FALSE FALSE  TRUE FALSE FALSE  TRUE
## [421] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [428] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
## [435]  TRUE FALSE FALSE  TRUE FALSE FALSE FALSE
## [442]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## [449]  TRUE FALSE FALSE  TRUE FALSE FALSE  TRUE
## [456] FALSE FALSE FALSE  TRUE FALSE FALSE  TRUE
## [463] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [470]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
## [477] FALSE FALSE  TRUE FALSE FALSE  TRUE FALSE
## [484] FALSE  TRUE FALSE  TRUE FALSE FALSE  TRUE
## [491] FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
## [498] FALSE FALSE  TRUE FALSE  TRUE FALSE FALSE
## [505] FALSE  TRUE FALSE FALSE
```

To obtain the indexes, one can use R's function `which`

```
which(find_peaks(sun.spct$s.e.irrad))

##   [1]  23  25  29  35  38  40  43  48  51  53  55
##  [12]  58  62  68  72  74  78  86  89  93  95  99
##  [23] 103 110 112 117 120 122 124 127 129 134 141
##  [34] 144 150 152 156 159 165 169 172 174 176 180
##  [45] 183 186 188 190 196 198 201 203 207 211 214
##  [56] 217 220 224 226 230 233 237 239 244 246 253
##  [67] 255 258 260 263 266 269 271 273 276 278 281
##  [78] 285 290 295 299 302 305 308 313 316 320 323
##  [89] 327 329 335 337 341 343 346 350 359 361 370
## [100] 376 382 396 400 405 412 417 420 430 435 438
## [111] 442 449 452 455 459 462 470 479 482 485 487
## [122] 490 493 500 502 506
```

1.3.2 Obtaining the location of peaks as a wavelength in nanometres

Function `get_peaks` takes two numeric vectors as as arguments, x is, for spectra assumed to be a vector of wavelengths, and y the spectral variable to search for local maxima.

```
with(sun.spct, get_peaks(w.length, s.e.irrad))

##      x         y label
## 1  321 0.1822031   321
## 2  330 0.3295190   330
## 3  335 0.3129253   335
## 4  340 0.3352353   340
## 5  343 0.3380052   343
## 6  347 0.3207918   347
## 7  350 0.3453572   350
## 8  354 0.3758625   354
## 9  360 0.3707068   360
## 10 366 0.4491898   366
## 11 370 0.4393233   370
## 12 378 0.4969714   378
## 13 381 0.4362110   381
## 14 385 0.3915446   385
## 15 391 0.4822105   391
```

```
## 16 395 0.4699886   395
## 17 402 0.6497388   402
## 18 409 0.6615421   409
## 19 412 0.6742498   412
## 20 416 0.6761818   416
## 21 421 0.6701269   421
## 22 426 0.6388873   426
## 23 436 0.7336607   436
## 24 442 0.7188581   442
## 25 451 0.8204633   451
## 26 457 0.7984935   457
## 27 461 0.7711277   461
## 28 468 0.7665312   468
## 29 472 0.7693357   472
## 30 475 0.7724634   475
## 31 478 0.7869773   478
## 32 482 0.7832759   482
## 33 490 0.7728111   490
## 34 495 0.7899872   495
## 35 506 0.7701737   506
## 36 509 0.7466557   509
## 37 512 0.7510876   512
## 38 516 0.7302733   516
## 39 525 0.7376088   525
## 40 531 0.7603297   531
## 41 536 0.7429248   536
## 42 545 0.7272464   545
## 43 552 0.7178863   552
## 44 555 0.7117599   555
## 45 563 0.6991590   563
## 46 568 0.6750915   568
## 47 573 0.6713390   573
## 48 577 0.6644287   577
## 49 582 0.6853736   582
## 50 597 0.6256272   597
## 51 600 0.6372767   600
## 52 605 0.6614323   605
## 53 612 0.6468436   612
## 54 621 0.6464099   621
## 55 638 0.6233510   638
## 56 642 0.6138918   642
## 57 653 0.5819163   653
## 58 662 0.5995383   662
## 59 668 0.5977089   668
## 60 674 0.5879885   674
## 61 692 0.5029201   692
## 62 697 0.5164799   697
## 63 704 0.5013394   704
## 64 712 0.5070675   712
## 65 722 0.4345295   722
## 66 727 0.3855997   727
## 67 734 0.4676589   734
## 68 744 0.5006212   744
## 69 747 0.5025733   747
## 70 751 0.5000141   751
## 71 754 0.5007593   754
## 72 774 0.4746771   774
## 73 777 0.4716414   777
## 74 782 0.4680026   782
```

```
## 75 794 0.4213304   794
## 76 798 0.4236281   798
```

The returned value is a (shorter) data frame with two numeric vectors, x and y, and an optional chracter variables `label`, for each local maximum found in y.

> Methods for spectral objects will be added.

1.4 Task: Refining the location of peaks and valleys

The functions described in the previous section locate the observation with the locally highest y-value. This is in most cases the true location of the peaks as they may fall in between two observations along the wavelength axis. By fitting a suitable model to describe the shape of the peak, which is the result of the true peak and the slit function of the spectrometer, the true location of a peak can be approximated more precisely. There is no universally useful model, so we show some examples of a possible method of peak-position refinement.

In this example, in the second statement we refine the location of the shortest-wavelength peak found by `get_peaks` in the first statement. For this approach to work, the peaks should be clearly visible, and not very close to each other. We use the spectral irradiance measured from a UV-B lamp as an example.

```
stepsize(philips.tl01.bentham.spct)

## [1] 0.5 0.5

peaks <- with(philips.tl01.bentham.spct, get_peaks(w.length, s.e.irrad, span = 51))
fit <- nls(s.e.irrad ~ d + a1*exp(-0.5*((w.length-c1)/b1)^2),
           start=list(a1=6, b1=1, c1=peaks[1, 1], d=0), data=philips.tl01.bentham.sp
fit

## Nonlinear regression model
##   model: s.e.irrad ~ d + a1 * exp(-0.5 * ((w.length - c1)/b1)^2)
##    data: philips.tl01.bentham.spct
##        a1        b1        c1         d
##   6.08259   0.90542 311.64836   0.03093
##  residual sum-of-squares: 7.684
##
## Number of iterations to convergence: 8
## Achieved convergence tolerance: 3.682e-06

fit$m$getPars()[["c1"]]

## [1] 311.6484

peaks[1, 1]

## [1] 311.5
```

Because in this example the spectral resolution of the data is high, the improvement is small. We now subsample the spectral data, and repeat the calculations.

```
my.tl01.spct <- subset(philips.tl01.bentham.spct, w.length %% 2 == 0)
stepsize(my.tl01.spct)

## [1] 2 2

my.peaks <- with(my.tl01.spct, get_peaks(w.length, s.e.irrad, span = 51))
my.fit <- nls(s.e.irrad ~ d + a1*exp(-0.5*((w.length-c1)/b1)^2),
           start=list(a1=6, b1=1, c1=my.peaks[1, 1], d=0), data=my.tl01.spct)
my.fit

## Nonlinear regression model
##   model: s.e.irrad ~ d + a1 * exp(-0.5 * ((w.length - c1)/b1)^2)
##    data: my.tl01.spct
##        a1        b1        c1         d
##   4.36981   0.91409 311.85914   0.03175
##  residual sum-of-squares: 0.1554
##
## Number of iterations to convergence: 4
## Achieved convergence tolerance: 1.956e-07

my.fit$m$getPars()[["c1"]]

## [1] 311.8591

my.peaks[1, 1]

## [1] 312
```

1.5 Task:

Part III

Catalogue of data sources

Part IV

Data acquisition and modelling

CHAPTER 2

Further reading about R

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APPENDIX A

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 3.2.0 (2015-04-16)
## 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] methods   tools     stats     graphics
```

```
## [5] grDevices utils     datasets  base
##
## other attached packages:
##  [1] photobiologyLamps_0.3.0
##  [2] photobiologygg_0.3.3
##  [3] scales_0.2.4
##  [4] ggplot2_1.0.1
##  [5] proto_0.3-10
##  [6] photobiologyWavebands_0.3.1.9000
##  [7] photobiology_0.6.7.90000
##  [8] data.table_1.9.4
##  [9] stringr_1.0.0
## [10] knitr_1.10.5
##
## loaded via a namespace (and not attached):
##  [1] Rcpp_0.11.6      magrittr_1.5
##  [3] MASS_7.3-40      munsell_0.4.2
##  [5] colorspace_1.2-6 splus2R_1.2-0
##  [7] highr_0.5        plyr_1.8.2
##  [9] caTools_1.17.1   grid_3.2.0
## [11] gtable_0.1.2     digest_0.6.8
## [13] reshape2_1.4.1   formatR_1.2
## [15] bitops_1.0-6     memoise_0.2.1
## [17] evaluate_0.7     stringi_0.4-1
## [19] lubridate_1.3.3  chron_2.3-45
```