R4Photobiology

A Suite of R Packages

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Outline

Photobiology

Definition, tasks, problems

- **Photobiology** is the study of responses to visible and ultraviolet radiation in living organisms.
- Typical tasks:
  - Describe and quantify the light environment.
  - Describe and quantify the responses of organisms to light.
  - Compute summary radiation quantities meaningful for different processes.
- Many calculations are conceptually simple but computations complex.

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Light-related spectra

What is common to all these spectra?

- A variable **wavelength**, λ, (or equivalent quantity) is always present
- Some other quantity either *expressed per unit wavelength* or as a ratio is also present
- Wavelength is a continuous variable, but measurements are taken at discrete and rather frequently arbitrary positions along this axis.
- The response variable is also a continuous variable and in most cases variation along the wavelength axis is also continuous.

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Example calculation

(Energy) irradiance

$$I_{\lambda_{min}\ldots\lambda_{max}} = \int_{\lambda=\lambda_{min}}^{\lambda=\lambda_{max}} I(\lambda)\mathrm{d}\lambda \qquad (1)$$

where $I_{\lambda_{min}\ldots\lambda_{max}}$ is irradiance in $\mathrm{W\,m^{-2}}$ for a *waveband*, λ is wavelength in nanometres, $I(\lambda)$ is the spectral irradiance in $\mathrm{W\,m^{-2}\,nm^{-1}}$, and λ_{min} and λ_{max} are the boundaries of the waveband (region) integrated.

Although this is a simple operation, practical problems (e.g. for Excel user) are:

1. $I(\lambda)$ is available only at discrete values of λ
2. *step* size of λ values is variable within a single measurement
3. $I(\lambda)$ may need to be interpolated at the boundaries of the waveband

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Example calculation

Weighted (energy) irradiance

$$I_w = \int_{\lambda=\lambda_{\min}}^{\lambda=\lambda_{\max}} I(\lambda) \times w(\lambda) \mathrm{d}\lambda \qquad (2)$$

where I_w is an *effective* irradiance in *weighted* $\mathrm{W\,m^{-2}}$, λ is wavelength in nanometres, $I(\lambda)$ is the spectral irradiance in $\mathrm{W\,m^{-2}\,nm^{-1}}$, $w(\lambda)$ is a dimensionless **spectral weighting function** (SWF).

Additional practical problems are:

...

1. **SWFs**, $w(\lambda)$, can be either defined as functions or tabulated multipliers
2. **SWFs** are frequently discontinuous
3. **SWFs** outside a specified range of wavelengths are assumed to be equal to zero or to be undefined, depending on the case

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Aims: clean and friendly ‘programmatic’ interface

- Hide the need of interpolation from users.
- Use an integration scheme over wavelengths not affected by irregular spacing of observations.
- Use a consistent way for describing operations and operands.
- Support reproducible research approaches.
- *Reasonably* fast performance.

Aims: help prevent user errors

- Define a class system that keeps track of different types of spectral data and their metadata.
- Provide functions for conversions among bases of expression.
- Provide functions for conversions among related quantities.
- Save data and metadata (e.g. units of expression) in same object.
- Propagate (and merge) comments and other metadata contained in objects when feasible.
- Use specialized *operators* for calculations involving spectral objects.

Aims: make sanity checks easy

- Provide a good set of “reference” data for comparisons.
- Make it easy to combine such data to predict outcomes...
- ...e.g. light-source emission spectra and filter transmission spectra.
- Make it easy to plot different types of spectra.
- Make it easy to meaningfully annotate such plots.

History

Development stages

Stage 00: ≈ 1998 Started playing with R.

Stage 0: 2000– R became the system I use by default.

Stage 1: 2011–2012 Collected functions from existing scripts used in my research group.

Stage 2: 2012–2013 Used a “prototype” version of my photobiology package in two training events.

Stage 3: 2013 Improved performance (because we had a set of half million spectra to analyse).

Stage 4: 2014–2015 Simplified user interface for teaching and general use.

Satge 5: 2015–2016 Write book or handbook on photobiological calculations using R.

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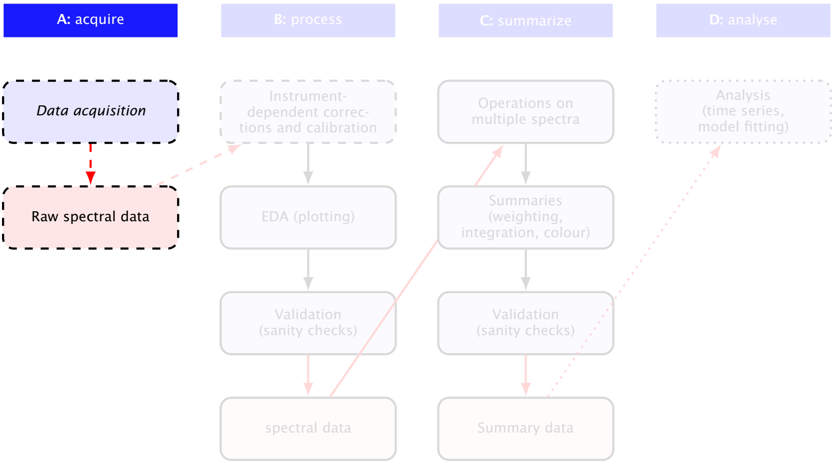
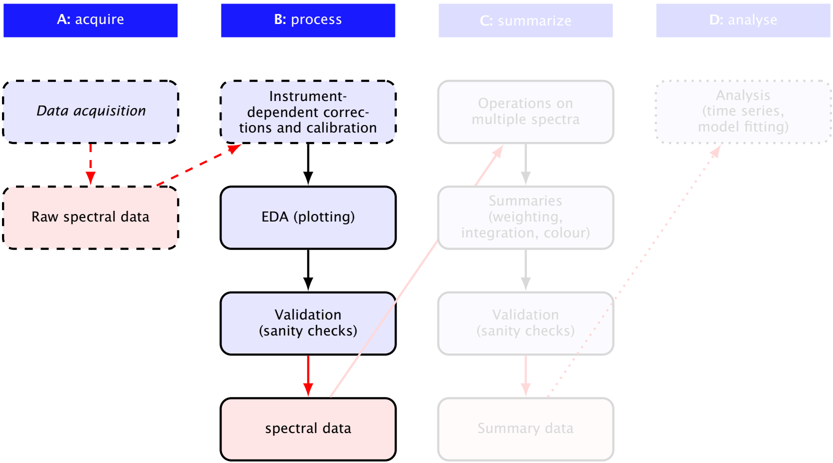
Data flow

First look



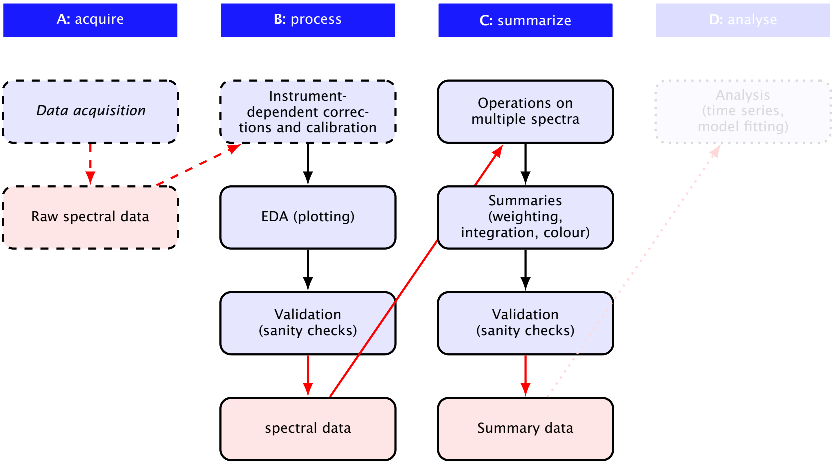
Data flow

First look



Data flow

First look



Data flow

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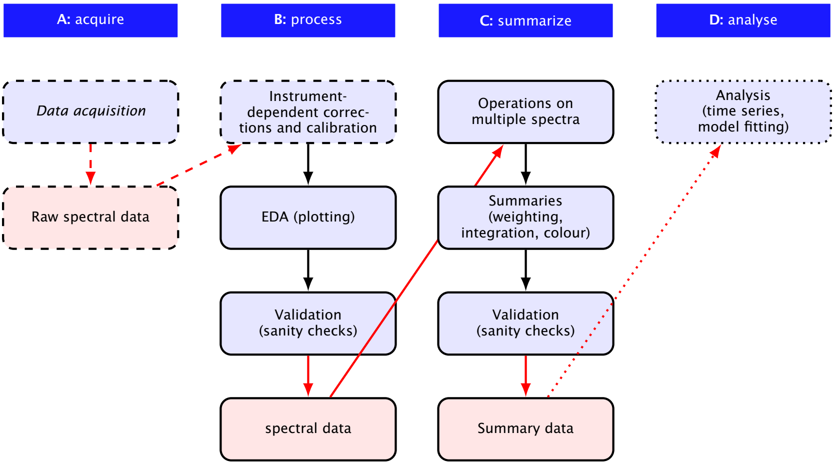


B: Example data

Spectral irradiance of sunlight

```
sun.spct

##       w.length     s.e.irrad
##   1:       293 2.609665e-06
##   2:       294 6.142401e-06
##   3:       295 2.176175e-05
##  ---
## 506:       798 4.236281e-01
## 507:       799 4.185850e-01
## 508:       800 4.069055e-01
```

`w.length` = wavelength in namometres (10^{-9} m, 1 nm = 10 Å)
`s.e.irrad` = spectral energy irradiance in $\mathrm{W\,m^{-2}\,nm^{-1}}$

B: Example data

Transmittance of a glass filter from Schott

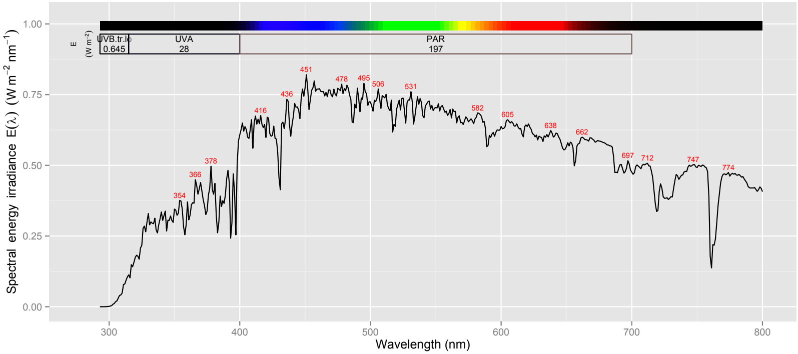
```
gg400.spct

##      w.length   Tfr
##   1:      200 1e-05
##   2:      210 1e-05
##   3:      220 1e-05
##  ---
## 178:     5050 1e-05
## 179:     5100 1e-05
## 180:     5150 1e-05
```

`w.length` = wavelength in namometres (10^{-9} m, 1 nm = 10 Å)
`Tfr` = spectral transmittance as a fraction of one

B: plot methods for spectra

A sunlight spectrum

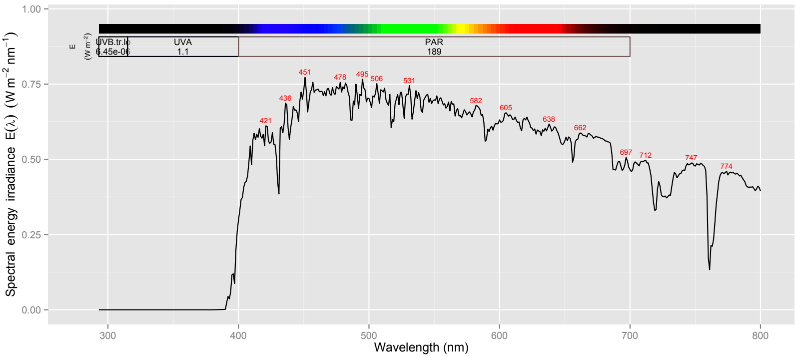
```
plot(sun.spct)
```



C: Operators for spectra

e.g. using operators to simulate spectral irradiance under a filter

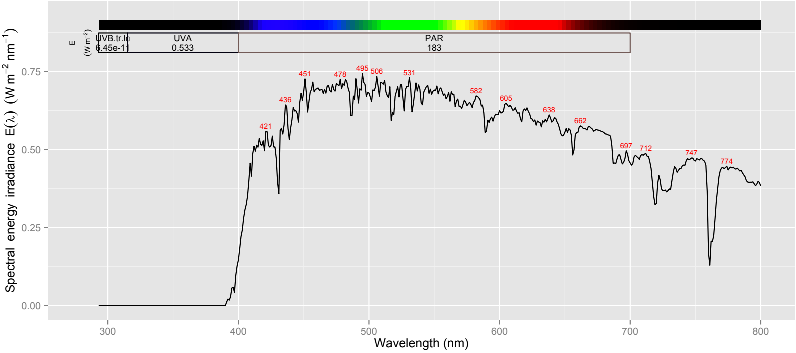
```r
plot(sun.spct * gg400.spct)
```



C: Operators for spectra

e.g. using operators to simulate the effect of two stacked filters

```
plot(sun.spct * gg400.spct^2)
```



C: Summaries of spectra

summary, wavelength range, equivalent color definition

```
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

range(sun.spct)

## [1] 293 800

color(sun.spct)

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

C: Summaries of spectra

e.g. irradiance (integral over wavelengths): total

$$I_{\lambda_{\min}\ldots\lambda_{\max}} = \int_{\lambda=\lambda_{\min}}^{\lambda=\lambda_{\max}} I(\lambda)\,\mathrm{d}\lambda \tag{3}$$

```
irrad(sun.spct)

##    Total
## 269.1249
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: Summaries of spectra

e.g. irradiance (integral over wavelengths): ultraviolet-A

$$I_{\text{UV-A}} = \int_{\lambda=\text{start(UV-A)}}^{\lambda=\text{end(UV-A)}} I(\lambda)\,\mathrm{d}\lambda \tag{4}$$

```r
irrad(sun.spct, UVA())

##  UVA.ISO
## 27.98418
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: Summaries of spectra

e.g. weighted irradiance (integral over wavelengths): CIE erythemal (human skin reddening)

$$I_{\mathrm{CIE}} = \int_{\lambda=\mathrm{start}(w_{\mathrm{CIE}})}^{\lambda=\mathrm{end}(w_{\mathrm{CIE}})} I(\lambda) \times w_{\mathrm{CIE}}(\lambda) \mathrm{d}\lambda \quad (5)$$

```
irrad(sun.spct, CIE())

##  CIE98.298.tr.lo
##       0.08181415
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: Summaries of spectra

e.g. irradiance for the band(s) defined according to wavelengths in nanometres

```
irrad(sun.spct, waveband(c(400, 700)))

##  range.400.700
##       196.6343
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

```
irrad(sun.spct, split_bands(c(400, 500, 600, 700)))

##  range.400.500  range.500.600  range.600.700
##       69.69042       68.48951       58.45435
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

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C: Summaries of spectra

e.g. photon (quantum) irradiance for two bands and the corresponding photon ratio

```
q_irrad(sun.spct, list(Red(), Blue()))

##      Red.ISO     Blue.ISO
## 0.0004511084 0.0001490288
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

```
q_ratio(sun.spct, Red(), Blue())

##  Red.ISO: Blue.ISO(q:q)
##                3.026988
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

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## attr(,"radiation.unit")
## [1] "q:q ratio"
```

C: Summaries of spectra

e.g. simulating effect of a filter on irradiance

```
irrad(sun.spct, UVA())

##  UVA.ISO
## 27.98418
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

```
irrad(sun.spct * gg400.spct, UVA())

##  UVA.ISO
## 1.100092
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: Summaries of spectra

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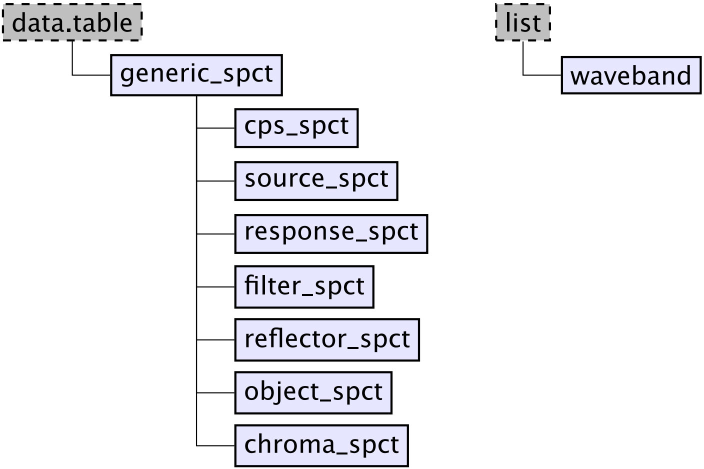
Classes

For spectral data and for wavebands



Classes

Class of returned objects

A filtered light source is a light source, not a filter:

```
class(gg400.spct * sun.spct)

## [1] "source_spct"  "generic_spct" "data.table"   "data.frame"
```

An attenuated light source is still a light source:

```
class(1/3 * sun.spct)

## [1] "source_spct"  "generic_spct" "data.table"   "data.frame"
```

A stack of two filters is still a filter:

```
class(gg400.spct * ug1.spct)

## [1] "filter_spct"  "generic_spct" "data.table"   "data.frame"
```

Attributes

```
getTimeUnit(sun.spct)

## [1] "second"
```

```
getTimeUnit(sun.daily.spct)

## [1] "day"
```

```
getTimeUnit(sun.daily.spct, force.duration = TRUE)

## [1] "86400s (~1 days)"
```

Attributes

```
getTimeUnit(sun.spct)

## [1] "second"
```

```
getTimeUnit(sun.daily.spct)

## [1] "day"
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getTimeUnit(sun.daily.spct, force.duration = TRUE)

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Attributes

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```

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getTimeUnit(sun.daily.spct)

## [1] "day"
```

```
getTimeUnit(sun.daily.spct, force.duration = TRUE)

## [1] "86400s (~1 days)"
```

Comments in data objects

Automatic comment in object after acquisition + calibration using R

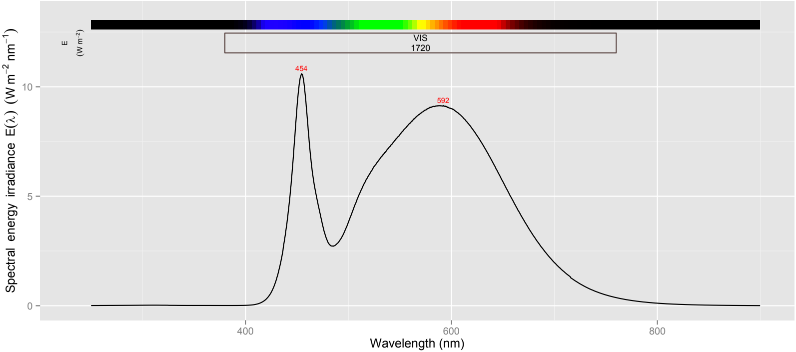
```
load("Lumitronix.cal.spcts.Rda")
cat(comment(Lumitronix_4cm.cal.spct))

## Spectrometer: MayaPro2000 s/n MAYP11278
## Bench with grating HC1, filter 000 and slit 010s
## Measured on 2015-05-19 18:23:34
## processed on 2015-05-19 with MayaCalc ver 3.2.3
## using HDR: TRUE, using NR: FALSE, method: full
## calibration dated (automatic): 2014-10-15
## number of scans          :      695,        86
## integration times (ms)  :     7.20,     58.53
## total times (s)          :   5.0040,    5.0334
## max counts               : 28410 out of 64000 (44%)
## LOW SIGNAL!
```

Plot same spectral data

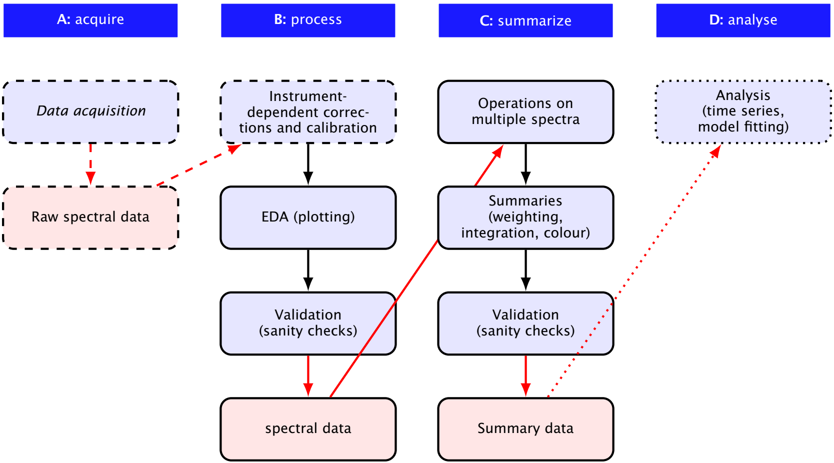
Automatically generated axis labels and summaries: Units are ‘known’

```
plot(Lumitronix_4cm.cal.spct, w.band = VIS())
```



Data flow

Second look



Where to find the suite of packages

- mailto:pedro.aphalo@helsinki.fi
- Web site at http://www.r4photobiology.info/
  - Installation instructions
  - Posts (also) RSS feed for package updates
  - Some other related posts and pages
  - Book/handbook early draft coming soon
- Packages not yet submitted to CRAN
- Own repository with CRAN-like structure at http://www.r4photobiology.info/R
- Git repository at Bitbucket http://bitbucket.org/aphalo/
- Other resources at http://www.uv4plants.org/

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- Packages not yet submitted to CRAN
- Own repository with CRAN-like structure at http://www.r4photobiology.info/R
- Git repository at Bitbucket http://bitbucket.org/aphalo/
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Where to find the suite of packages

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