R4Photobiology
A Suite of R Packages

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SenPEP

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http://blogs.helsinki.fi/senpep-blog/

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Outline

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2. Examples
3. Under the hood
4. Resources
5. Acknowledgements
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, \( \lambda \), (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

\[ I_{\lambda_{\text{min}}...\lambda_{\text{max}}} = \int_{\lambda=\lambda_{\text{min}}}^{\lambda=\lambda_{\text{max}}} I(\lambda) \, d\lambda \]  

where \( I_{\lambda_{\text{min}}...\lambda_{\text{max}}} \) is irradiance in \( \text{W m}^{-2} \) for a waveband, \( \lambda \) is wavelength in nanometres, \( I(\lambda) \) is the spectral irradiance in \( \text{W m}^{-2} \text{nm}^{-1} \), and \( \lambda_{\text{min}} \) and \( \lambda_{\text{max}} \) 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 \( \lambda \)
2. step size of \( \lambda \) values is variable within a single measurement
3. \( I(\lambda) \) may need to be interpolated at the boundaries of the waveband
Example calculation

(Energy) irradiance

\[
I_{\lambda_{\text{min}}...\lambda_{\text{max}}} = \int_{\lambda=\lambda_{\text{min}}}^{\lambda=\lambda_{\text{max}}} I(\lambda)\,d\lambda
\]  

(1)

where \(I_{\lambda_{\text{min}}...\lambda_{\text{max}}}\) is irradiance in \(W\,m^{-2}\) for a waveband, \(\lambda\) is wavelength in nanometres, \(I(\lambda)\) is the spectral irradiance in \(W\,m^{-2}\,nm^{-1}\), and \(\lambda_{\text{min}}\) and \(\lambda_{\text{max}}\) 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 \(\lambda\)
2. step size of \(\lambda\) values is variable within a single measurement
3. \(I(\lambda)\) may need to be interpolated at the boundaries of the waveband
Example calculation

Weighted (energy) irradiance

\[ I_w = \int_{\lambda=\lambda_{\text{min}}}^{\lambda=\lambda_{\text{max}}} I(\lambda) \times w(\lambda) \, d\lambda \]  

(2)

where \( I_w \) is an effective irradiance in weighted \( \text{W m}^{-2} \), \( \lambda \) is wavelength in nanometres, \( I(\lambda) \) is the spectral irradiance in \( \text{W m}^{-2} \text{ nm}^{-1} \), \( w(\lambda) \) 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
Example calculation

Weighted (energy) irradiance

\[ I_w = \int_{\lambda=\lambda_{\text{min}}}^{\lambda=\lambda_{\text{max}}} I(\lambda) \times w(\lambda) \, d\lambda \]  \hspace{1cm} (2)

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Additional practical problems are:

\[ \begin{align*}
1 & \textbf{SWFs, } w(\lambda), \text{ can be either defined as functions or tabulated multipliers} \\
2 & \textbf{SWFs} \text{ are frequently discontinuous} \\
3 & \textbf{SWFs} \text{ outside a specified range of wavelengths are assumed to be equal to zero or to be undefined, depending on the case}
\end{align*} \]
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: \(\approx 1998\)  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 5: 2015–2016  Write book or handbook on photobiological calculations using R.
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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.
Stage 5: 2015–2016  Write book or handbook on photobiological
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Data flow
First look

A: acquire

Data acquisition

B: process

Instrument-dependent corrections and calibration

EDA (plotting)

Validation (sanity checks)

spectral data

C: summarize

Operations on multiple spectra

Summaries (weighting, integration, colour)

Validation (sanity checks)

Summary data

D: analyse

Analysis (time series, model fitting)
Data flow

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*Data acquisition*

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### Examples

B: Example data

Spectral irradiance of sunlight

```r
sun.spct

```sun.spct```

```r
# 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 \(Wm^{-2}nm^{-1}\)
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 nanometres \((10^{-9} \text{ m}, 1 \text{ nm} = 10 \text{ Å})\)

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

```
plot(sun.spct * gg400.spct)
```
C: Operators for spectra

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

```r
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

\[ I_{\lambda_{\text{min}}...\lambda_{\text{max}}} = \int_{\lambda=\lambda_{\text{min}}}^{\lambda=\lambda_{\text{max}}} I(\lambda) \, d\lambda \]  

\texttt{irrad(sun.spct)}

```r
## 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

\[ I_{UV-A} = \int_{\lambda=start(UV-A)}^{\lambda=end(UV-A)} I(\lambda) d\lambda \]  \hspace{1cm} (4)

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

```r
## 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)

\[ I_{\text{CIE}} = \int_{\lambda=\text{start}(w_{\text{CIE}})}^{\lambda=\text{end}(w_{\text{CIE}})} I(\lambda) \times w_{\text{CIE}}(\lambda) d\lambda \] (5)

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

```text
## 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

```r
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

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irrad(sun.spct, waveband(c(400, 700)))
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## 196.6343
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irrad(sun.spct, split_bands(c(400, 500, 600, 700)))
## range.400.500 range.500.600 range.600.700
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## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
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```
C: Summaries of spectra

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

\[
q_{\text{irrad}}(\text{sun.spct, } \text{list(Red(), Blue()))})
\]

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

\[
q_{\text{ratio}}(\text{sun.spct, Red(), Blue()})
\]

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

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C: Summaries of spectra

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

```r
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"
```

```r
q_ratio(sun.spct, Red(), Blue())
## Red.ISO: Blue.ISO(q:q)
## 3.026988
## 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

E.g. simulating effect of a filter on irradiance

```r
irrad(sun.spct, UVA())
## UVA.ISO
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```
Classes

For spectral data and for wavebands

- data.table
  - generic_spct
    - cps_spct
    - source_spct
    - response_spct
    - filter_spct
    - reflector_spct
    - object_spct
    - chroma_spct

- list
  - waveband
Classes
Class of returned objects

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

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

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

An attenuated light source is still a light source:

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

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

A stack of two filters is still a filter:

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

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

```r
getTimeUnit(sun.spct)

## [1] "second"
```

```r
gTimeUnit(sun.daily.spct)

## [1] "day"
```

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

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

```r
getTimeUnit(sun.spct)
## [1] "second"

getTimeUnit(sun.daily.spct)
## [1] "day"

getTimeUnit(sun.daily.spct, force.duration = TRUE)
## [1] "86400s (~1 days)"
```
Attributes

```r
getTimeUnit(sun.spct)
## [1] "second"
```

```r
getTimeUnit(sun.daily.spct)
## [1] "day"
```

```r
getTimeUnit(sun.daily.spct, force.duration = TRUE)
## [1] "86400s (~1 days)"
```
Comments in data objects
Automatic comment in object after acquisition + calibration using R

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

```r
## 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!
```
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Under the hood

Plot same spectral data
Automatically generated axis labels and summaries: Units are ‘known’

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

![Graph showing spectral energy irradiance (W m^(-2) nm^(-1)) vs. wavelength (nm). Peaks at 454 and 592 nm, with a summarized VIS band.]
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Analysis (time series, model fitting)
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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- 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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Members of my research group and collaborators (most of them listed below).


A new umbrella organization at our campus.

My employer.

For funding, decisions 252548, 16775.

EU for funding COST action FA0906 ‘UV4Growth’ and our training events and meetings.

Equipment suppliers *Ocean Optics, sglux, Schott* for support and/or providing technical data on their products for inclusion as examples.
A very special thanks to the R and \TeX{} communities for all the tools, packages, documentation and help that made developing this suite not only possible but also so enjoyable!

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{spectrum.png}
\caption{Spectral energy irradiance (W m$^{-2}$ nm$^{-1}$) across different wavelengths.}
\end{figure}

\textbf{Thanks for listening!}