A handbook of theory and recipes

R for Photobiology

Theory and recipes for common calculations

Pedro J. Aphalo
Andreas Albert
T. Matthew Robson
Titta Kotilainen

Helsinki, 29 July 2016

Available through Leanpub

Typeset with XeLaTeX in Lucida Bright and Lucida Sans using the KOMA-Script book class.
The manuscript was written using R with package 'knitr'. The manuscript was edited in WinEdt and RStudio. The source files for the whole book are available at https://bitbucket.org/aphalo/using-r.

Contents

List of Tables

List of Figures

List of Text Boxes

Preface

This is the draft of a handbook that accompanies the release of the suite of R packages for photobiology (r4photobiology). The biophysical theory needed to follow the examples is concisely described in Part I, but the treatment is very concise(**Bjoern2015**). Methods for research in the UV photobiology of plants (**Aphalo2012**) covers theory and practice of experimentation in photobiology. The software used in the examples including a suite of R packages developed by one of the authors is described in Part II. A cookbook with recipes for different calculation tasks is in Part III. Part IV includes three chapters dedicated to reading and writing data in *foreign* formats, including direct acquisition from measuring instruments. Part V gives a brief overview of the data sets included in the suite. Although this text includes many different recipes, it is not comprehensive in covering all the functionality of the packages. The packages themselves include *User Guides* and help pages describing their functionality in detail. A series of articles describing specific aspects of the use of the suite is being published in the UV4Plants Bulletin.

This handbook assumes that readers are already familiar with the R language and in Part I that they are familiar with Physics and Mathematics, including calculus and geometry.

1 Typographical conventions

Code examples are typeset in monospaced font and syntax highlighted in colour. References to R language elements—i.e. R 'code'—in the main text are also in a `monospaced` font but in black on a faint background. Package names are typeset between single quotes in a 'sans serif' font.

We use the icon exemplified in the page margin next to this paragraph to highlight contents that require special attention because they are frequent causes of errors and problems.

We use the icon exemplified in the page margin next to this paragraph to highlight contents that is advanced and will require the reader to linger on it to get a deep understanding—and which can, alternatively, be skipped on first reading by those readers which want a faster path to learning to do simpler calculations.

2 Acknowledgements

We thank Stefano Catola, Paula Salonen, David Israel, Neha Rai, Tendry Randriamanana, Saara Harkikainen, Christian Bianchi-Strømme and …for very useful comments and suggestions on the draft manuscript and examples used in training schools. The friendly and generous R community also deserves a big 'Thank you!'.

Helsinki, July 2016.

The authors.

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	absorptance (%).
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	reflectance (%).
σ	Stefan-Boltzmann constant.
τ	transmittance (%).
χ	water vapour content in the air ($\mathrm{g\,m^{-3}}$).
A	absorbance (absorbance units).
ANCOVA	analysis of covariance.
ANOVA	analysis of variance.
BSWF	biological spectral weighting function.
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 (**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 ($\mathrm{kJ\,m^{-2}\,d^{-1}}$).
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	photosynthetically active radiation, 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	proportional-integral-derivative (control algorithm).
PMMA	polymethylmethacrylate.
PPFD	photosynthetic photon flux density, 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	radiation amplification factor (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 ($\lambda = 100$–400 nm).
UV-A	ultraviolet-A radiation ($\lambda = 315$–400 nm).
UV-B	ultraviolet-B radiation ($\lambda = 280$–315 nm).
UV-C	ultraviolet-C radiation ($\lambda = 100$–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

Theory behind calculations

1

Radiation properties

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)
library(ggplot2)
library(ggspectra)
library(photobiologyWavebands)
library(photobiologySun)
library(photobiologyLamps)
library(photobiologyLEDs)
```

1.2 Ultraviolet and visible radiation

From the viewpoint of Physics, ultraviolet (UV) and visible (VIS) radiation are both considered electromagnetic waves and are described by Maxwell's equations.[1] The wavelength ranges of UV and visible radiation and their usual names are listed in Table 1.1. The long wavelengths of solar radiation, called infrared (IR) radiation, are also listed. The colour ranges indicated in Table 1.1 are an approximation as different individual human observers will not perceive colours exactly in the same way. We follow the ISO definitions for wavelength boundaries for colours (**??**). Other finer-grained colour name series are also in use (**Aphalo2012**)). The electromagnetic spectrum is continuous with no clear boundaries between one colour and the next, the colours could be thought as artifacts produced by our sensory system, and are meaningful only from the perspective of an *average* human observer. Especially in the IR region the subdivision is somewhat arbitrary and the boundaries used in the literature vary.

Radiation can also be thought of as composed of quantum particles or photons. The energy of a quantum of radiation in a vacuum, q, depends on the wavelength, λ, or frequency[2], ν,

$$q = h \cdot \nu = h \cdot \frac{c}{\lambda} \tag{1.1}$$

with the Planck constant $h = 6.626 \times 10^{-34}$ J s and speed of light in vacuum $c = 2.998 \times 10^{8}$ m s^{-1}. When dealing with numbers of photons, the equation (1.1) can be extended by using Avogadro's number $N_{\mathrm{A}} = 6.022 \times 10^{23}$ mol^{-1}. Thus, the energy of one mole of photons, q', is

$$q' = h' \cdot \nu = h' \cdot \frac{c}{\lambda} \tag{1.2}$$

[1] These equations are a system of four partial differential equations describing classical electromagnetism.

[2] 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 1.1.

with $h' = h \cdot N_A = 3.990 \times 10^{-10}$ J s mol^{-1}. Example 1: red light at 600 nm has about 200 kJ mol^{-1}, therefore, 1 μmol photons has 0.2 J. Example 2: UV-B radiation at 300 nm has about 400 kJ mol^{-1}, therefore, 1 μmol photons has 0.4 J. Equations 1.1 and 1.2 are valid for all kinds of electromagnetic waves (see Section **??** for a worked-out calculation example).

One way of understanding the relationship between the distance and positions of source and observer (or sensor) on the amount of radiation received is to use a geometric model. Bellow we describe such a model, in which a point source is located at the centre or origin of an imaginary sphere. As the distance from the origin increases, the surface area of the sphere at this distance increases. The relationship between the distance increase and area increase is, obviously, not linear. In addition, according to the well known cosine law, the amount of radiation received per unit area depends on the angle of incidence. This informal description, will is formally described below.

When a beam or the radiation passing into a space or sphere is analysed, two important parameters are necessary: the distance to the source and the measuring position—i.e. if the receiving surface is perpendicular to the beam or not. The geometry is illustrated in Figure 1.1 with a radiation source at the origin. The radiation is received at distance r by a surface of area dA, tilted by an angle α to the unit sphere's surface element, so called solid angle, dΩ, which is a two-dimensional angle in a space. The relation between dA and dΩ in spherical coordinates is geometrically explained in Figure 1.1.

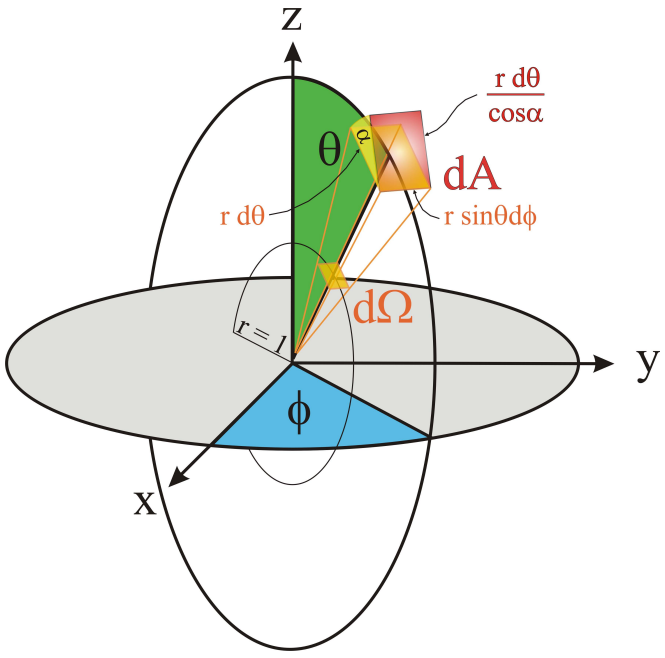


Figure 1.1: Definition of the solid angle dΩ and the geometry of areas in the space (redrawn after **bergm33**), where the given solid angle dΩ remains the same, regardless of distance r, while the exposed area exemplified by dA will change with distance r from the origin (light source) and the angle α, if the exposed area (or detector) is tilted. The angle denoted by ϕ is the azimuth angle and θ is the zenith angle.

Table 1.1: Regions of the electromagnetic radiation spectrum according to different authorities, standards or in common use. The use of what we have called *medical* and *common* definitions of the UV bands should be avoided, as it makes interpretation of experimental results and comparison of radiation quantities with studies using the accepted international standard very difficult. ISO 21348 (**ISO21348:2007**), BTV (**Aphalo2012**), Smith (**Smith1981a**), Sellaro (**Sellaro2010**).

Waveband name	Wavelength range (nm)					
	ISO 21348	BTV	Smith	Sellaro	*medical*	*common*
UV	$100 \leq \lambda < 400$	$100 \leq \lambda < 400$				
UVC	$100 \leq \lambda < 280$	$100 \leq \lambda < 280$			$220 \leq \lambda < 290$	$200 \leq \lambda < 280$
UVB	$280 \leq \lambda < 315$	$280 \leq \lambda < 315$			$290 \leq \lambda < 320$	$280 \leq \lambda < 320$
UVA	$315 \leq \lambda < 400$	$315 \leq \lambda < 400$				$320 \leq \lambda < 400$
VIS	$380 \leq \lambda < 760$					
Purple (Violet)	$360 \leq \lambda < 450$	$400 \leq \lambda < 455$				
Blue	$450 \leq \lambda < 500$	$455 \leq \lambda < 492$		$420 \leq \lambda < 490$		
Green	$500 \leq \lambda < 570$	$492 \leq \lambda < 577$		$500 \leq \lambda < 570$		
Yellow	$570 \leq \lambda < 591$	$577 \leq \lambda < 597$				
Orange	$591 \leq \lambda < 610$	$597 \leq \lambda < 622$				
Red	$610 \leq \lambda < 760$	$622 \leq \lambda < 700$	$655 \leq \lambda < 665$	$620 \leq \lambda < 680$		
Far red		$(700 \leq \lambda < 770)$	$725 \leq \lambda < 735$	$700 \leq \lambda < 750$		
IR-A (near IR)	$760 \leq \lambda < 1400$	$770 \leq \lambda < 3000$				
IR-B (mid IR)	$1400 \leq \lambda < 3000$	$3000 \leq \lambda < 50000$				
IR-C (far IR)	$3000 \leq \lambda < 10^6$	$50000 \leq \lambda < 10^6$				

The solid angle is calculated from the zenith angle θ and azimuth angle ϕ, which denote the direction of the radiation beam

$$\mathrm{d}\Omega = \mathrm{d}\theta \cdot \sin\theta \mathrm{d}\phi \tag{1.3}$$

The area of the receiving surface is calculated by a combination of the solid angle of the beam, the distance r from the radiation source and the angle α of the tilt:

$$\mathrm{d}A = \frac{r\mathrm{d}\theta}{\cos\alpha} \cdot r\sin\theta\mathrm{d}\phi \tag{1.4}$$

which can be rearranged to

$$\Rightarrow \mathrm{d}A = \frac{r^2}{\cos\alpha} \quad \mathrm{d}\Omega \tag{1.5}$$

Thus, the solid angle is given by

$$\Omega = \int_A \frac{\mathrm{d}A \cdot \cos\alpha}{r^2} \tag{1.6}$$

The unit of the solid angle is a steradian (sr). The solid angle of an entire sphere is calculated by integration of equation (1.3) over the zenith (θ) and azimuth (ϕ) angles, $0 \leq \theta \leq \pi(180^\circ)$ and $0 \leq \phi \leq 2\pi(360^\circ)$, and is 4π sr. For example, the sun or moon seen from the Earth's surface appear to have a diameter of about 0.5° which corresponds to a solid angle element of about 6.8×10^{-5} sr.

When radiation travels through a medium it can be absorbed (the energy 'taken up' by the material's atoms) or scattered (the direction of travel of the radiation randomly altered). Both of these phenomena affect the amount of radiation that reaches the 'other end of the path' where the observer or sensor is located, and their effect depends on the length of the path. Once again, this informal description, is stated formally below.

The processes responsible for the variation of the radiance $L(\lambda, \theta, \phi)$ as the radiation beam travels through any kind of material, are primarily absorption a and scattering b, which are called inherent optical properties, because they depend only on the characteristics of the material itself and are independent of the light field. Radiance is added to the directly transmitted beam, coming from different directions, due to elastic scattering, by which a photon changes direction but not wavelength or energy level. An example of this is Raleigh scattering in very small particles, which causes the scattering of light in a rainbow. A further gain of radiance into the direct path is due to inelastic processes like fluorescence, where a photon is absorbed by the material and reemitted as a photon with a longer wavelength and lower energy level, and Raman scattering. The elastic and inelastic scattered radiance is denoted as L^E and L^I, respectively. Internal sources of radiances, L^S, like bioluminescence of biological organisms or cells contribute also to the detected radiance. The path of the radiance through a thin horizontal layer with thickness $\mathrm{d}z = z_1 - z_0$ is shown schematically in Figure 1.2.

Putting all this together, the radiative transfer equation is

$$\cos\theta \frac{\mathrm{d}L}{\mathrm{d}z} = -(a+b) \cdot L + L^E + L^I + L^S \tag{1.7}$$

The dependencies of L on λ, θ, and ϕ are omitted here for brevity. No exact analytical solution to the radiative transfer equation exists, hence it is necessary either to use

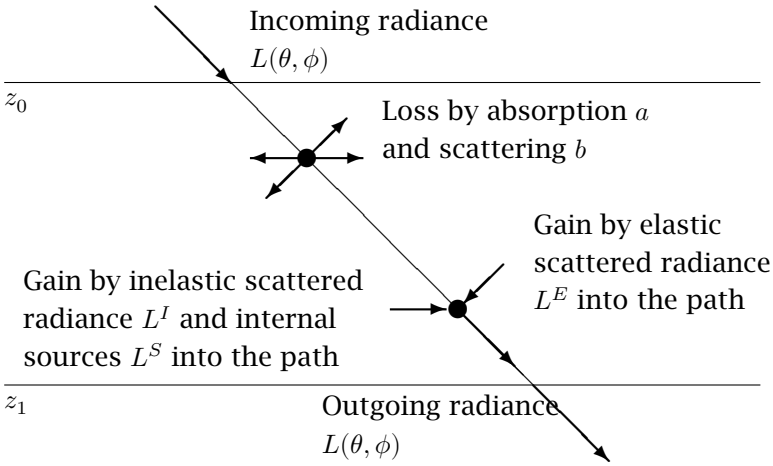


Figure 1.2: Path of the radiance and influences of absorbing and scattering particles in a thin homogeneous horizontal layer of air or water. The layer is separated from other layers of different characteristics by boundary lines at height z_0 and z_1.

numerical models or to make approximations and find an analytical parametrisation. A numerical model is for example the Monte Carlo method. The parameters of the light field can be simulated by modelling the paths of photons. For an infinite number of photons the light field parameters reach their exact values asymptotically. The advantage of the Monte Carlo method is a relatively simple structure of the program, and it simulates nature in a straightforward way, but its disadvantage is the time-consuming computation involved. Details of the Monte Carlo method are explained for example by (**prahl89**), (**Wang1995**)[3], or (**moble94**).

The other way to solve the radiative transfer equation is through the development of analytical parameterisations by making approximations for all the quantities needed. In this case, the result is not exact, but it has the advantage of fast computing and the analytical equations can be inverted just as fast. This leads to the idealised case of a source-free ($L^S = 0$) and non-scattering media, i.e. $b = 0$ and therefore $L^E = L^I = 0$. Then, equation 1.7 can be integrated easily and yields

$$L(z_1) = L(z_0) \cdot \mathrm{e}^{-\frac{a \cdot (z_1 - z_0)}{\cos\theta}} \tag{1.8}$$

The boundary value $L(z_0)$ is presumed known. This result is known as Beer's law (or Lambert's law, Bouguer's law, Beer-Lambert law), denotes any instance of exponential attenuation of light and is exact only for purely absorbing media—i.e. media that do not scatter radiation. It is of direct application in analytical chemistry, as it describes the direct proportionality of absorbance (A) to the concentration of a coloured solute in a transparent solvent.

Different physical quantities are used to describe the "amount of radiation" and their definitions and abbreviations are listed in Table 1.2. Taking into account Equation 1.6 and assuming a homogenous flux, the important correlation between irradi-

[3]Their program is available from the website of Oregon Medical Laser Center at http://omlc.ogi.edu/software/mc/

Table 1.2: Physical quantities of light.

Symbol	Unit	Description
$\Phi = \frac{\partial q}{\partial t}$	W = J s^{-1}	Radiant flux: absorbed or emitted energy per time interval
$H = \frac{\partial q}{\partial A}$	J m^{-2}	Exposure: energy towards a surface area. (In plant research this is called usually *dose* (H), while in Physics *dose* refers to absorbed radiation.)
$E = \frac{\partial \Phi}{\partial A}$	W m^{-2}	Irradiance: flux or radiation towards a surface area, radiant flux density
$I = \frac{\partial \Phi}{\partial \Omega}$	W sr^{-1}	Radiant intensity: emitted radiant flux of a surface area per solid angle
$\epsilon = \frac{\partial \Phi}{\partial A}$	W m^{-2}	Emittance: emitted radiant flux per surface area
$L = \frac{\partial^2 \Phi}{\partial \Omega (\partial A \cdot \cos \alpha)} = \frac{\partial I}{\partial A \cdot \cos \alpha}$	W m^{-2} sr^{-1}	Radiance: emitted radiant flux per solid angle and surface area depending on the angle between radiant flux and surface perpendicular

ance E and intensity I is

$$E = \frac{I \cdot \cos \alpha}{r^2} \tag{1.9}$$

The irradiance decreases by the square of the distance to the source and depends on the tilt of the detecting surface area. This is valid only for point sources. For outdoor measurements the sun can be assumed to be a point source. For artificial light sources simple LEDs (light-emitting diodes) without optics on top are also effectively point sources. However, LEDs with optics—and other artificial light sources with optics or reflectors designed to give a more focused dispersal of the light—deviate to various extents from the rule of a decrease of irradiance proportional to the square of the distance from the light source.

Besides the physical quantities used for all electromagnetic radiation, there are also equivalent quantities to describe visible radiation, so called photometric quantities. The human eye as a detector led to these photometric units, and they are commonly used by lamp manufacturers to describe their artificial light sources. See Box **??** on page **??** for a short description of these quantities and units.

Photometric quantities

In contrast to (spectro-)radiometry, where the energy of any electromagnetic radiation is measured in terms of absolute power (J s = W), photometry measures light as perceived by the human eye. Therefore, radiation is weighted by a luminosity function or visual sensitivity function describing the wavelength dependent response of the human eye. Due to the physiology of the eye, having rods and cones as light receptors, different sensitivity functions exist for the day (photopic vision) and night (scotopic vision), $V(\lambda)$ and $V'(\lambda)$, respectively. The maximum response during the day is at $\lambda = 555$ nm and during night at $\lambda = 507$ nm. Both response functions (normalised to their maximum) are shown in Figure 1.3 as established by the Commission Internationale de l'Éclairage (CIE, International Commission on Illumination, Vienna, Austria) in 1924 for photopic vision and 1951 for scotopic vision (**Schwiegerling2004**). The data are available from the Colour and Vision Research Laboratory at `http://www.cvrl.org`. Until now, $V(\lambda)$ is the basis of all photometric measurements.

Corresponding to the physical quantities of radiation summarized in the table 1.2, the equivalent photometric quantities are listed in the table below and have the subscript v. The ratio between the (physiological) luminous flux Φ_v and the (physical) radiant flux Φ is the (photopic) photometric equivalent $K(\lambda) = V(\lambda) \cdot K_m$ with $K_m = 683$ lm W^{-1} (lumen per watt) at 555 nm. The dark-adapted sensitivity of the eye (scotopic vision) has its maximum at 507 nm with 1700 lm W^{-1}. The base unit of luminous intensity is candela (cd). One candela is defined as the monochromatic intensity at 555 nm (540 THz) with $I = \frac{1}{683}$ W sr^{-1}. The luminous flux of a normal candle is around 12 lm. Assuming a homogeneous emission into all directions, the luminous intensity is about $I_\mathrm{v} = \frac{12\ \mathrm{lm}}{4\pi\ \mathrm{sr}} \approx 1$ cd.

Photon or quantum quantities of radiation.

When we are interested in photochemical reactions, the most relevant radiation quantities are those expressed in photons. The reason for this is that, as discussed in section **??** on page **??**, molecules are excited by the absorption of certain fixed amounts of energy or quanta. The surplus energy "decays" by non-photochemical processes. When studying photosynthesis, where many photons of different wavelengths are simultaneously important, we normally use photon irradiance to describe amount of PAR. The name photosynthetic photon flux density, or PPFD, is also frequently used when referring to PAR photon irradiance. When dealing with energy balance of an object instead of photochemistry, we use (energy) irradiance. In meteorology both UV and visible radiation, are quantified using energy-based quantities. When dealing with UV photochemistry as in responses mediated by UVR8, an UV-B photoreceptor, the use of quantum quantities is preferred. According to the physical energetic quantities in the table 1.2, the equivalent photon related quantities are listed in the table below and have the subscript p.

These quantities can be also used based on a 'chemical' amount of moles by dividing the quantities by Avogadro's number $N_A = 6.022 \times 10^{23}$ mol^{-1}. To determine a quantity in terms of photons, an energetic quantity has to be weighted by the number of photons, i.e. divided by the energy of a single photon at each wavelength as

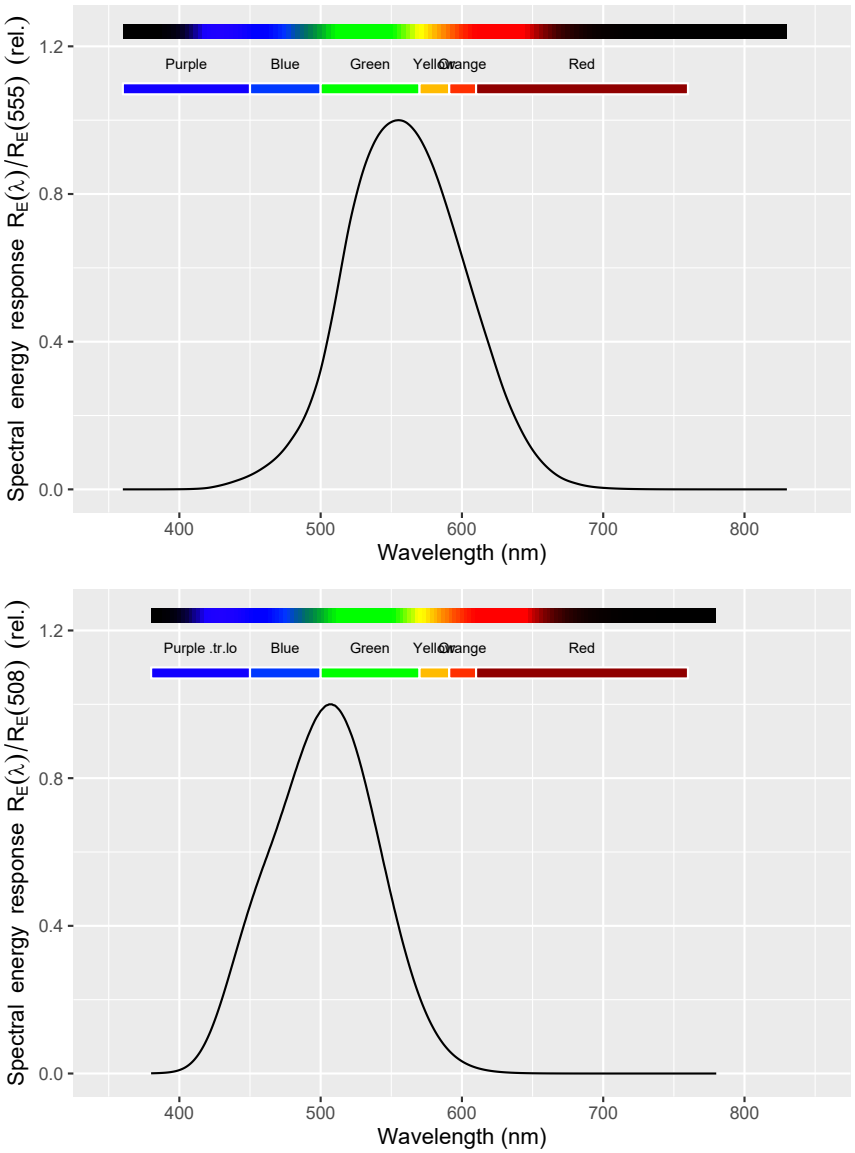


Figure 1.3: Relative spectral intensity of human colour sensation during day (solid line) and night (dashed line), $V(\lambda)$ and $V'(\lambda)$ respectively.

defined in equation 1.1. This yields for example

$$\Phi_\mathrm{p} = \frac{\lambda}{h\,c} \cdot \frac{\partial q}{\partial t} \qquad \text{and} \qquad Q(\lambda) = \frac{\lambda}{h\,c} \cdot E(\lambda)$$

Table 1.3: Photometric quantities of light.

Symbol	Unit	Description
q_v	lm s	Luminous energy or quantity of light
$\Phi_\mathrm{v} = \frac{\partial q_\mathrm{v}}{\partial t}$	lm	Luminous flux: absorbed or emitted luminous energy per time interval
$I_\mathrm{v} = \frac{\partial \Phi_\mathrm{v}}{\partial \Omega}$	cd = lm sr^{-1}	Luminous intensity: emitted luminous flux of a surface area per solid angle
$E_\mathrm{v} = \frac{\partial \Phi_\mathrm{v}}{\partial A}$	lux = lm m^{-2}	Illuminance: luminous flux towards a surface area
$\epsilon_\mathrm{v} = \frac{\partial \Phi_\mathrm{v}}{\partial A}$	lux	Luminous emittance: luminous flux per surface area
$H_\mathrm{v} = \frac{\partial q_\mathrm{v}}{\partial A}$	lux s	Light exposure: quantity of light towards a surface area
$L_\mathrm{v} = \frac{\partial^2 \Phi_\mathrm{v}}{\partial \Omega (\partial A \cdot \cos\alpha)} = \frac{\partial I_\mathrm{v}}{\partial A \cdot \cos\alpha}$	cd m^{-2}	Luminance: luminous flux per solid angle and surface area depending on the angle between luminous flux and surface perpendicular

Table 1.4: Photon quantities of light.

Symbol	Unit	Description
Φ_p	s^{-1}	Photon flux: number of photons per time interval
$Q = \frac{\partial \Phi_\mathrm{p}}{\partial A}$	$\mathrm{m}^{-2}\ \mathrm{s}^{-1}$	Photon irradiance: photon flux towards a surface area, photon flux density (sometimes also symbolised by E_p)
$H_\mathrm{p} = \int_t Q\ \mathrm{d}t$	m^{-2}	Photon exposure: number of photons towards a surface area during a time interval, photon fluence

Photon or quantum quantities of radiation.

When dealing with bands of wavelengths, for example an integrated value like PAR from 400 to 700 nm, it is necessary to repeat these calculations at each wavelength and then integrate over the wavelengths. For example, the PAR photon irradiance or PPFD in moles of photons is obtained by

$$\mathrm{PPFD} = \frac{1}{N_\mathrm{A}} \int_{400\ \mathrm{nm}}^{700\ \mathrm{nm}} \frac{\lambda}{hc}\, E(\lambda)\, \mathrm{d}\lambda$$

For integrated values of UV-B or UV-A radiation the calculation is done analogously by integrating from 280 to 315 nm or 315 to 400 nm, respectively.

If we have measured (energy) irradiance, and want to convert this value to photon irradiance, the exact conversion will be possible only if we have information about the spectral composition of the measured radiation. Conversion factors at different wavelengths are given in the table below. For PAR, 1 $\mathrm{W\,m^{-2}}$ of "average daylight" is approximately 4.6 $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$. This is exact only if the radiation is equal from 400 to 700 nm, because the factor is the value at the central wavelength at 550 nm. Further details are discussed in section **??** on page **??**.

Table 1.5: Conversion factors of photon and energy quantities at different wavelengths.

	$\mathrm{W\,m^{-2}}$ to $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$	λ (nm)
	2.34	280
UV-B	2.49	298
	2.63	315
UV-A	2.99	358
	3.34	400
PAR	4.60	550
	5.85	700

There are, in principle, two possible approaches to measuring radiation. The first is to observe light from one specific direction or viewing angle, which is the radiance L. The second is to use a detector, which senses radiation from more than one direction and measures the so-called irradiance E of the entire sphere or hemisphere. The correlation between irradiance E and radiance L of the wavelength λ is given by integrating over all directions of incoming photons.

$$E_0(\lambda) = \int_\Omega L(\lambda,\Omega)\mathrm{d}\Omega \tag{1.10}$$

$$E(\lambda) = \int_\Omega L(\lambda,\Omega)|\cos\alpha|\mathrm{d}\Omega \tag{1.11}$$

Depending on the shape of a detector (which may be either planar or spherical) the irradiance is called (plane) irradiance E or fluence rate (also called scalar irradiance) E_0. A planar sensor detects incoming photons depending on the incident angle and a spherical sensor detects all photons equally weighted for all directions. See section **??** on page **??** for a more detailed discussion.

Here we have discussed the properties of light based on energy quantities. In photobiology there are good reasons to quantify radiation based on photons. See Box **??** on page **??**, and section **??** on page **??**.

1.3 Solar radiation

When dealing with solar radiation, we frequently need to describe the position of the sun. The azimuth angle (ϕ) is measured clockwise from the North on a horizontal plane. The position on the vertical plane is measured either as the zenith angle (θ) downwards from the zenith, or as an elevation angle (h) upwards from the horizon. Consequently $h+\theta = 90^\circ = \frac{\pi}{2}$ radians. See Figure 1.4 for a diagram. In contrast to Figure

1.1 and the discussion in section **??** where the point radiation source is located at the origin of the system of coordinates, when describing the position of the sun as in Figure 1.4 the observer is situated at the origin.

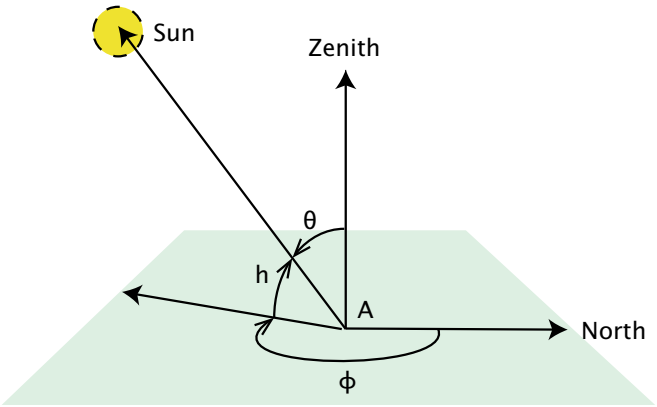


Figure 1.4: Position of the sun in the sky and the different angles used for its description by an observer located at point A. The azimuth angle is ϕ, the elevation angle is h and the zenith angle is θ. These angles are measured on two perpendicular planes, one horizontal and one vertical.

Ultraviolet and visible radiation are part of solar radiation, which reaches the Earth's surface in about eight minutes (t = time, r_0 = distance sun to earth, c = velocity of light in vacuum):

$$t = \frac{r_0}{c} \approx \frac{150 \times 10^9 \text{ m}}{3 \times 10^8 \frac{\text{m}}{\text{s}}} = 500 \text{ s} = 8.3 \text{ min}$$

The basis of all passive measurements is the incoming solar radiation, which can be estimated from the known activity of the sun ('productivity of photons'), that can be approximated by the emitted spectral radiance (L_s) described by Planck's law of black body radiation at temperature T, measured in degrees Kelvin (K):

$$L_\text{s}(\lambda, T) = \frac{2hc^2}{\lambda^5} \cdot \frac{1}{\text{e}^{(hc/k_\text{B}T\lambda)} - 1} \tag{1.12}$$

with Boltzmann's constant $k_\text{B} = 1.381 \times 10^{-23}$ JK^{-1}. The brightness temperature of the sun can be determined by Wien's displacement law, which gives the peak wavelength of the radiation emitted by a blackbody as a function of its absolute temperature

$$\lambda_{max} \cdot T = 2.898 \times 10^6 \,\text{nm K} \tag{1.13}$$

This means that for a maximum emission of the sun at about 500 nm the temperature of the sun surface is about 5800 K. The spectral irradiance of the sun $E_\text{s}(\lambda)$ can be estimated assuming a homogeneous flux and using the correlation of intensity I and radiance L from their definitions in table 1.2. The intensity of the sun $I_\text{s}(\lambda)$ is given by the radiance $L_\text{s}(\lambda)$ multiplied by the apparent sun surface (a non-tilted disk of radius $r_s = 7 \times 10^5$ km). To calculate the decreased solar irradiance at the moment of reaching the Earth's atmosphere, the distance of the sun to the Earth ($r_0 = 150 \times 10^6$ km) has

to be taken into account due to the inverse square law of irradiance of equation (1.9). Thus, the extraterrestrial solar irradiance is

$$E_{\mathrm{s}}(\lambda) = L_{\mathrm{s}}(\lambda) \cdot \frac{\pi r_s^2}{r_0^2} \tag{1.14}$$

Remembering the solid angle of equation (1.6), the right multiplication factor represents the solid angle of the sun's disk as seen from the Earth's surface ($\approx 6.8 \times 10^{-5}$ sr). Figure 1.5 shows the spectrum of the measured extraterrestrial solar radiation (Wehrli, 1985)[4] and the spectrum calculated by equation 1.14 using Planck's law of equation 1.12 at a black body temperature of 5800 K. Integrated over all wavelengths, E_{s} is about 1361 to 1362 $\mathrm{W\,m^{-2}}$ at top of the atmosphere (**Kopp2011**). This value is called the 'solar constant'. In former times, depending on different measurements, E_{s} varies by a few percent (**iqbal83**). For example, the irradiance at the top of the atmosphere (the integrated value) changes by ± 50 $\mathrm{W\,m^{-2}}$ (3.7 %) during the year due to distance variation caused by orbit excentricity (**moble94**). More accurate measurements during the last 25 years by spaceborne radiometers show a variability of the solar radiation of a few tenth of a percent. A detailed analysis is given by (**froeh04**). E_{s} can also be calculated by the Stefan-Boltzmann Law: the total energy emitted from the surface of a black body is proportional to the fourth power of its temperature. For an isotropically emitting source (Lambertian emitter), this means

$$L = \frac{\sigma}{\pi} \cdot T^4 \tag{1.15}$$

with the Stefan-Boltzmann constant $\sigma = 5.6705 \times 10^{-8}$ W m^{-2} K^{-4}. With $T = 5800$ K equation 1.15 gives the radiance of the solar disc. From this value, we can obtain an approximation of the solar constant, by taking into account the distance from the Earth to the Sun and the apparent size of the solar disc (see equations 1.6 and 1.9).

The total solar irradiance covers a wide range of wavelengths. Using some of the 'colours' introduced in table 1.1, table 1.6 lists the irradiance and fraction of E_{s} of different wavelength intervals.

Table 1.6: Distribution of the extraterrestrial solar irradiance E_{s} constant in different wavelength intervals calculated using the data of (**wehrl85**) shown in Figure 1.5.

Colour	Wavelength (nm)	Irradiance ($\mathrm{W\,m^{-2}}$)	Fraction of E_{s} (%)
UV-C	100 – 280	7	0.5
UV-B	280 – 315	17	1.2
UV-A	315 – 400	84	6.1
VIS	400 – 700	531	38.9
near IR	700 – 1 000	309	22.6
mid and far IR	$> 1\,000$	419	30.7
total		1 367	100.0

The extraterrestrial solar spectrum differs from that at ground level due to the absorption of radiation by the atmosphere, because the absorption peaks of water,

[4] Available as ASCII file at PMODWRC, ftp://ftp.pmodwrc.ch/pub/publications/pmod615.asc

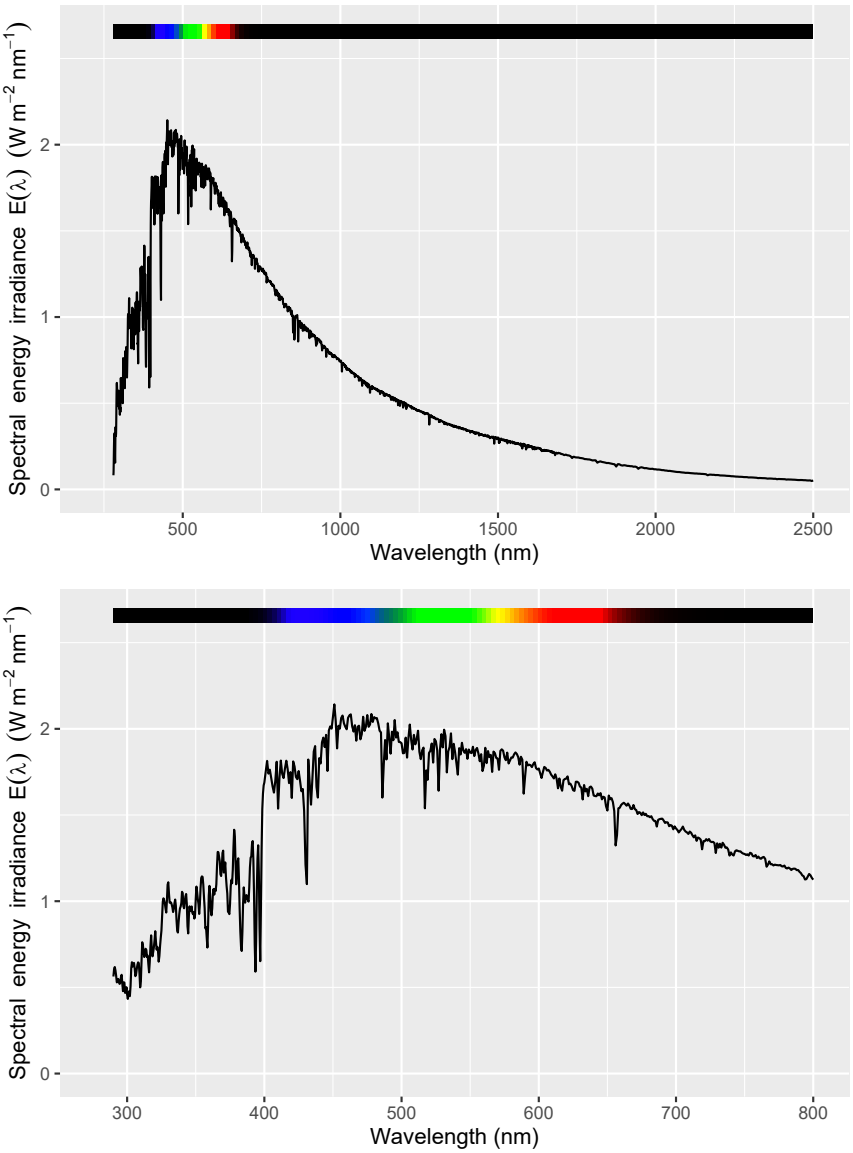


Figure 1.5: Extraterrestrial solar spectrum after (**Gueymard2004**). Contrast with Fig. 1.6.

CO_2 and other components of the atmosphere, cause corresponding valleys to appear in the solar spectrum at ground level. For example, estimates from measurements of the total global irradiance at Helmholtz Zentrum München (11.60° E, 48.22° N, 490 m above sea level) on two sunny days (17th April 1996, sun zenith angle of 38° and 27th May 2005, 27°) result in about 5% for wavelengths below 400 nm, about 45% from 400 to 700 nm, and about 50% above 700 nm. In relation to plant research, only the coarse structure of peaks and valleys is relevant, because absorption spectra of pigments *in vivo* have broad peaks and valleys. However, the solar spectrum has a much finer structure, due to emission and absorption lines of elements, which is not observable with the spectroradiometers normally used in plant research.

At the Earth's surface, the incident radiation or *global radiation* has two components, direct radiation and scattered or 'diffuse' radiation. Direct radiation is radiation travelling directly from the sun, while diffuse radiation is that scattered by the atmosphere. Diffuse radiation is what gives the blue colour to the sky and white colour to clouds. The relative contribution of direct and diffuse radiation to global radiation varies with wavelength and weather conditions. The contribution of diffuse radiation is larger in the UV region, and in the presence of clouds (Figures **??** and 1.7).

Not only total irradiance, but also the wavelength distribution of the solar spectrum changes with the seasons of the year and time of day. The spectral wavelength distribution is also changed by the amount of UV-absorbing ozone in the atmosphere, known as the ozone column. Figure 1.8 shows how spectral irradiance changes throughout one day. When the whole spectrum is plotted using a linear scale the effect of ozone depletion is not visible, however, if we plot only the UV region (Figure 1.9) or use a logarithmic scale (Figure 1.10), the effect becomes clearly visible. In addition, on a log scale, it is clear that the relative effect of ozone depletion on the spectral irradiance at a given wavelength increases with decreasing wavelength.

Seasonal variation in UV-B irradiance has a larger relative amplitude than variation in PAR (Figure **??**). This causes a seasonal variation in the UV-B: PAR ratio (Figure **??**). In addition to the regular seasonal variation, there is random variation as a result of changes in clouds (Figure **??**). Normal seasonal and spatial variation in UV can be sensed by plants, and could play a role in their adaptation to seasons and/or their position in the canopy.

UV-B irradiance increases with elevation in mountains and with decreasing latitude (Figure 1.11) and is particularly high on high mountains in equatorial regions. This has been hypothesized to be a factor in the determination of the tree line[5] in these mountains (**Flenley1992**).

An increase in the UV-B irradiance is caused by depletion of the ozone layer in the stratosphere, mainly as a consequence of the release of chlorofluorocarbons (CFCs), used in cooling devices such as refrigerators and air conditioners, and in some spray cans (**Graedel1993**). The most dramatic manifestation of this has been the seasonal formation of an "ozone hole" over Antarctica. It is controversial whether a true ozone hole has already formed in the Arctic, but strong depletion has occurred in year 2011 (**Manney2011**) and atmospheric conditions needed for the formation of a "deep" ozone hole are not very different from those prevalent in recent years. Not so dramatic, but consistent, depletion has also been observed at mid-latitudes in both hemispheres. CFCs and some other halocarbons have been phased out following the Montreal agreement and later updates. However, as CFCs have a long half life in the

[5] *Tree line* is the highest elevation on a mountain slope at which tree species are naturally able to grow.

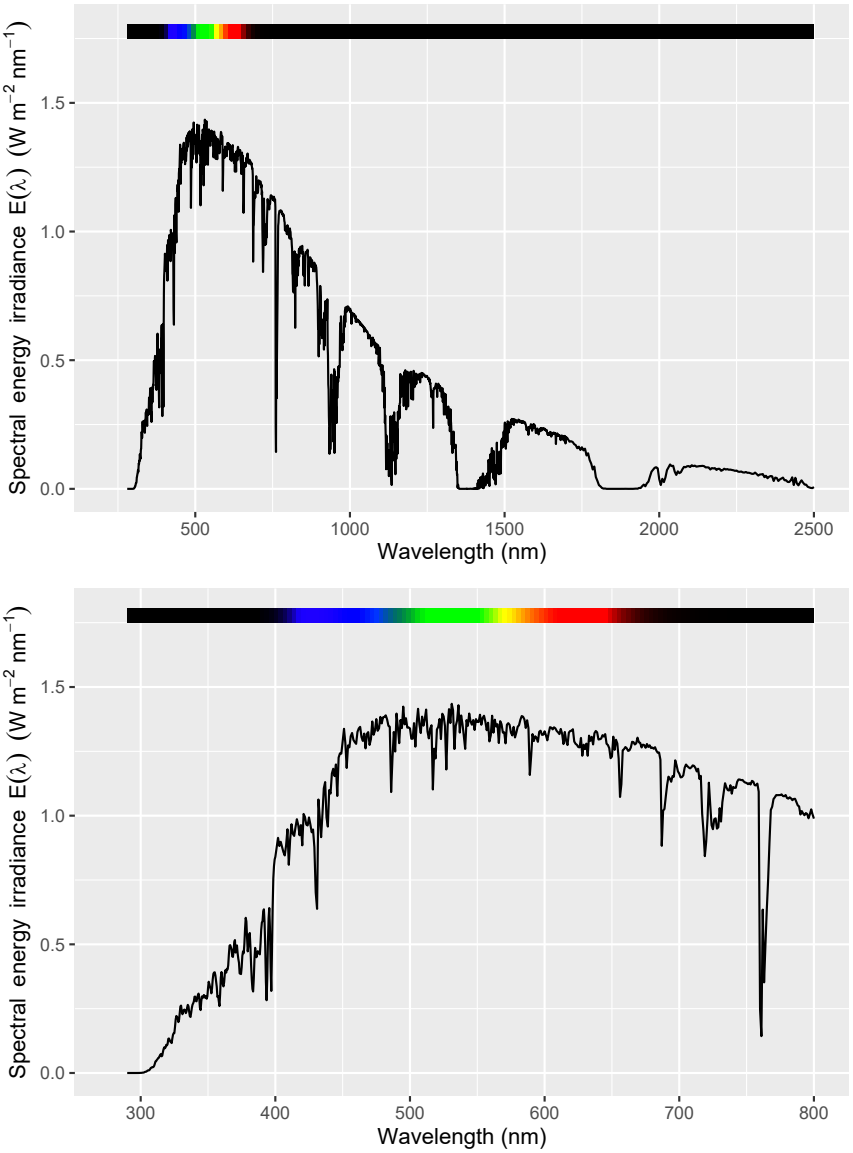


Figure 1.6: Ground level solar spectrum AM1.5 (1.5 air mass, solar zenith angle 48° 19′) according to ASTM G173-03 (**ASTM2003?**). Contrast with Fig. 1.5.

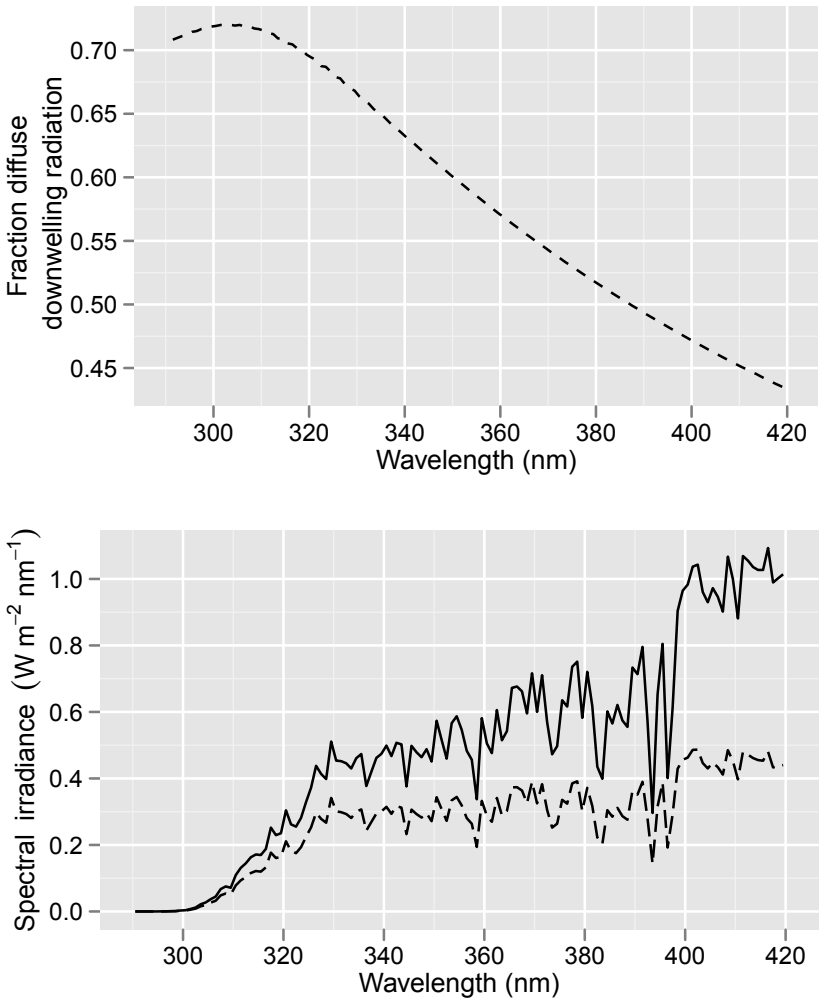


Figure 1.7: Diffuse component in solar UV. Spectral irradiance of total downwelling radiation (lower panel, solid line), diffuse downwelling radiation (lower panel, long dashes), and ratio of diffuse downwelling to total downwelling spectral irradiance (upper panel, dashed line) are shown. Data from TUV model (version 4.1) for solar zenith angle = $40°00'$, cloud-free conditions, 300 Dobson units. Simulations done with the Quick TUV calculator at `http://cprm.acd.ucar.edu/Models/TUV/Interactive_TUV/`.

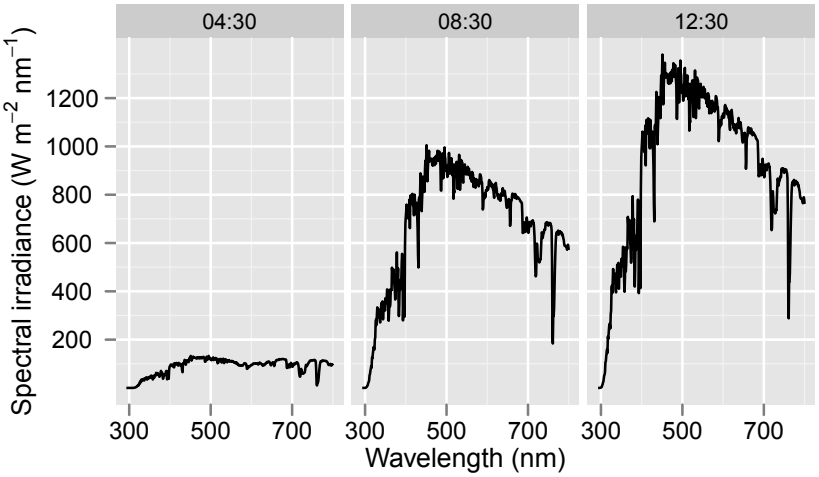


Figure 1.8: The solar spectrum through half a day. Simulations of global radiation (direct plus diffuse radiation) spectral irradiance on a horizontal surface at ground level) for a hypothetical 21 May with cloudless sky at Jokioinen (60°49'N, 23°30'E), under normal ozone column conditions. Effect of depletion is so small on the solar spectrum as a whole, that it would not visible in this figure. See (**Kotilainen2011**) for details about the simulations.

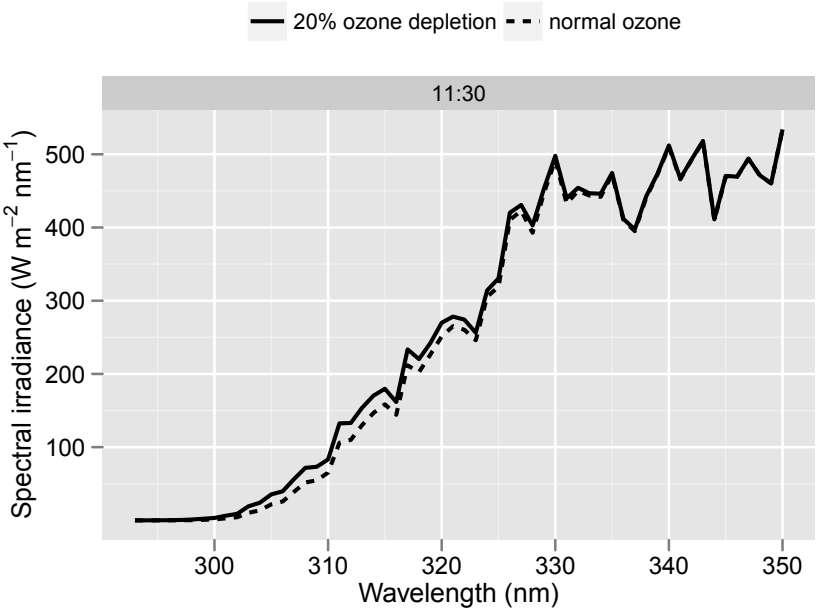


Figure 1.9: The effect of ozone depletion on the UV spectrum of global (direct plus diffuse) solar radiation at noon. See fig. 1.8 for details.

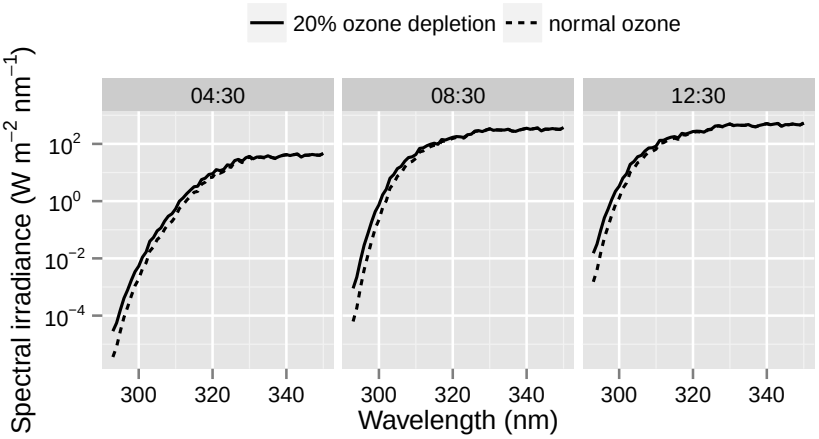


Figure 1.10: The solar UV spectrum through half a day. The effect of ozone depletion on global (direct plus diffuse) radiation. A logarithmic scale is used for spectral irradiance. See fig. 1.8 for details.

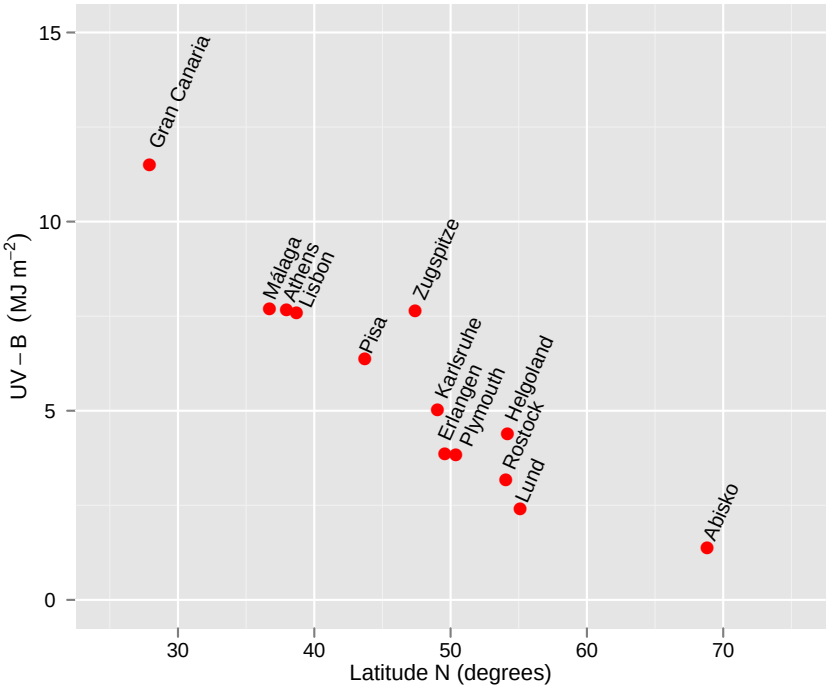


Figure 1.11: Latitudinal variation in UV-B radiation in the Northern hemisphere. UV-B annual exposure, measured with ELDONET instruments (**Haeder2007**).

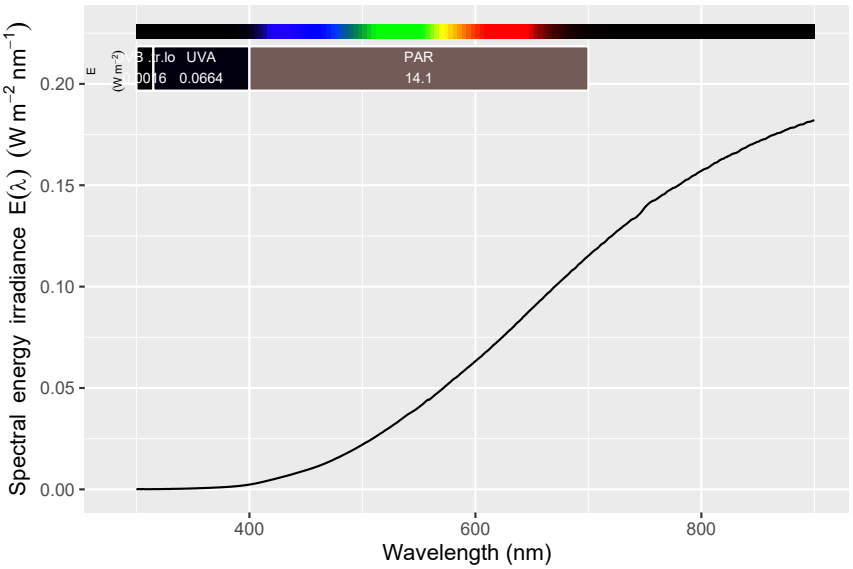


Figure 1.12: Spectral irradiance for a 60 W incandescent lamp

atmosphere, of the order of 100 years, their effect on the ozone layer will persist for many years, even after their use has been drastically reduced. Model-based predictions of changes in atmospheric circulation due to global climate change have been used to derive future trends in UV index and ozone column thickness (**Hegglin2009**). In addition, increased cloudiness and pollution, could lead to decreased UV and PAR, sometimes called 'global dimming' (**Stanhill2001**). It should be noted that, through reflection, broken clouds can locally increase UV irradiance to values above those under clear-sky conditions (**Frederick1993**; **Diaz1996**).

1.4 Artificial radiation

Different types of man-made VIS and UV radiation sources exist, based on exploiting different physical phenomena.

Incandescent light sources are "near-black bodies" heated at a very high temperature. Normal incandescent lamps are made from a Tungsten (also called Wolfram) wire heated at between 2500 and 3500 K by passing an electric current through it). The glass bulb enclosing it helps maintain the temperature and the low pressure inert gases filling it help slow down the evaporation of the metal (which can be seen in old lamps as a blackish deposit on the inside of glass bulb surface). These lamps produce a continuous spectrum (without well defined emission peaks), close to that from a true black body at the same temperature. Lamps with certain types of built-in reflectors may display a somewhat distorted spectrum as a result of interference or because of wavelength-selective properties (e.g. it is not unusual for lamps to have a reflector with high reflectivity for visible radiation but relatively high transmissivity for infra-red radiation).

Carbon arc lamps emit light by means of an electric "arc" between two carbon

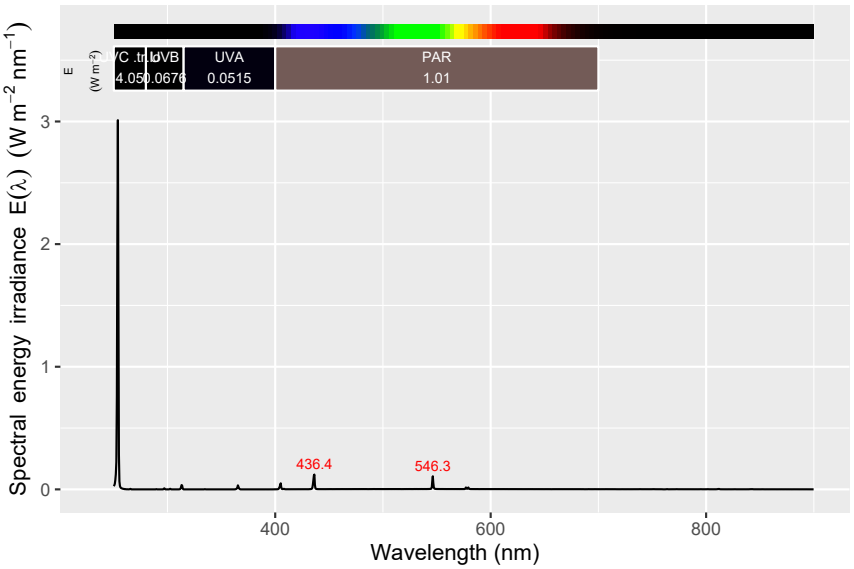


Figure 1.13: Spectral irradiance for a 'germicidal' low pressure mercury lamp.

electrodes, the arc heats the electrodes and carbon evaporates and because of its high temperature in-between the electrodes inducing light emission. The spectrum is broad but rather different to sunlight. Carbon arc lamps can be very bright and used in cinema projectors. They were invented before the incandescent tungsten lamp. Xenon arc lamps use Xenon gas enclosed in a special glass bulb. Xenon arc lamps have an emission spectrum rather similar to that of solar radiation, and together with UV-absorbing filters are frequently used in solar simulators. Some Xenon lamps do not emit continuously, such as modern "electronic" flashes used in photographic cameras. In such lamps the flash is produced by slowly charging a capacitor at a high voltage, and subsequently using this electrical charge to generate a short-lived arc in the lamp. Flash duration varies, but can be as short 0.1 ms in flashes used by photographers.

Other gas-discharge lamps use different gases or "vapours" or mixes of them. In these lamps, the elemental emission lines (corresponding to transitions between allowed energy states) are very well defined as long as the glass ampoule is not coated with special fluorescent compounds, and in many cases can be used as wavelength standards for calibration of spectrometers. The low pressure sodium lamps, easily recognizable by the orange light they emit, emit the same orange colour as that emitted by the flame of a gas ring in a cooker when water containing salt boils over from a pot. Low pressure mercury "vapour" lamps, such as germicidal ones made with an un-coated quartz-glass tube (technically called envelope) emit clearly at the know emission lines of mercury (Fig. 1.13). Being the container UV and VIS transmitting the strong line at 253.xx nm is very active as a germicidal agent. The "normal" fluorescent tubes used for illumination are enclosed in a tube coated with a so-called "phosphor" which absorbs UV radiation and re-emits it as visible radiation (Fig. 1.14). The spectrum of the emitted radiation is a combination of radiation emitted by the gaseous mercury, in particular those lines in the VIS region (e.g. 435.xx nm) and to some extent

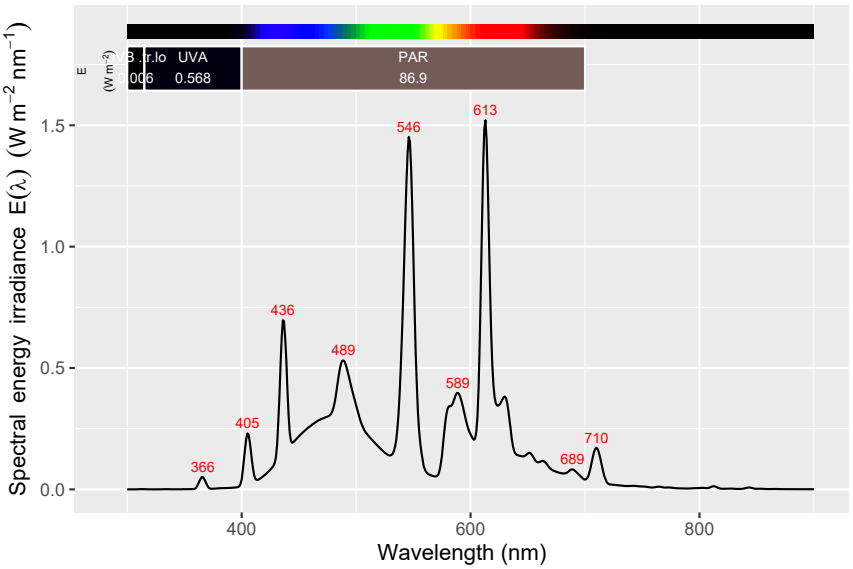


Figure 1.14: Spectral irradiance for a 'daylight', approx. 5200 K, fluorescent tube (Philips 36W 950).

in the UVA region, together with visible radiation re-emitted by the coating.

A more recent development is light generated by solid-state semiconductor devices or light-emitting diodes, once again light emission is the result of a transition between energy states of matter, but although emission takes place as a single peak, the peak is not as narrow or well defined as for elemental emission lines in discharge lamps (Fig. 1.15). Emission peaks have usually HFW of between 10 and 30 nm and their central wavelength may slightly shift depending on temperature and electrical current flowing through them. True LEDs always have a single peak of emission. White LEDs are based on a similar principle to that of fluorescent lamps: blue (or in some cases UVA) emitting LEDs are combined with a "phosphor" which absorbs in part the emitted radiation and re-emits the energy as radiation at longer wavelengths (Fig. 1.16). In some designs the phosphor is coated close to the semiconductor die, but in other cases, especially some arrays, the phosphor is in or on the encapsulating polymer. This coating in white LEDs looks yellow or orange when they are switched off.

Finally lasers, are different in that a laser is not another type of primary source of radiation. Lasing is a phenomenon which allows the generation of coherent radiation from a beam of incoherent radiation by means of a "cavity". Different primary sources of radiation can be used in lasers. In the case of laser diodes, an LED is the primary source of radiation. There are different possible types of cavities, for example gas-filled or solid state. Lasers are pulsed light sources, they do not emit continuously, although in many cases the frequency at which pulses are produced can be high. Even though laser pointers and other readily available lasers seem to us as being a continuous source of radiation, they are not. In fact, they are pulsed, and the duty cycle is low (pulses are brief compared to 'gaps') but each pulse has high energy. As radiation is in addition in a very narrow beam and almost of a single wavelength, a laser delivers spatially and temporarily concentrated energy pulses, that can make

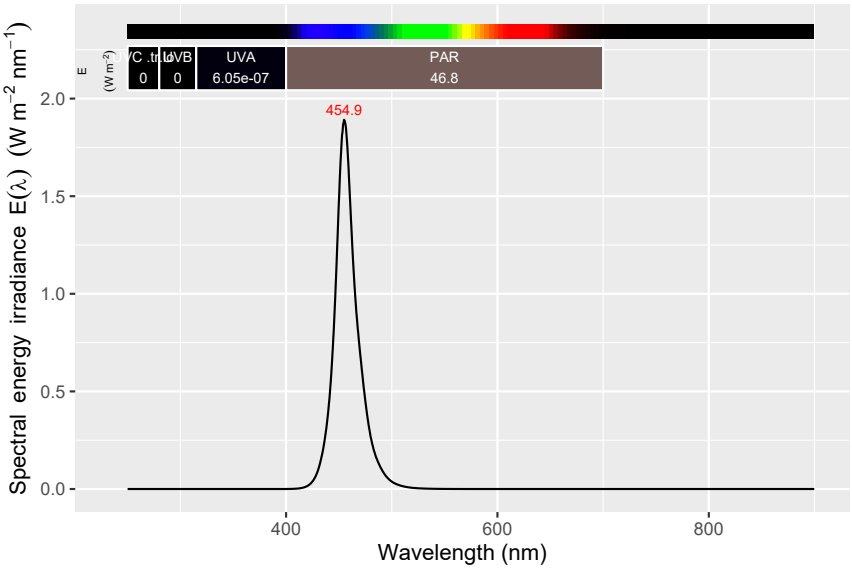


Figure 1.15: Spectral irradiance for a blue LED array (Huey Jann, 50 W).

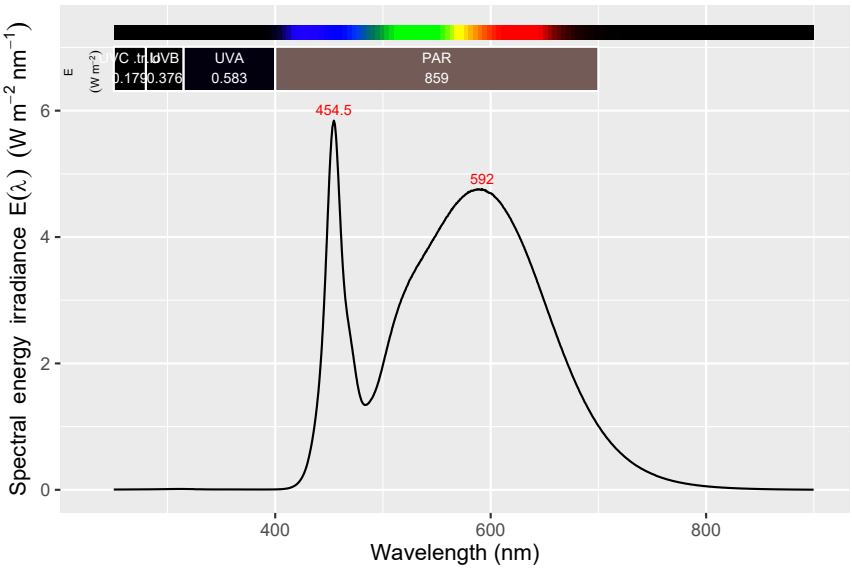


Figure 1.16: Spectral irradiance for 'neutral white LED', 4000 K, array (Lumitronix SmartArray Q36 LED-Module, 39W, using Nichia 757 LEDs).

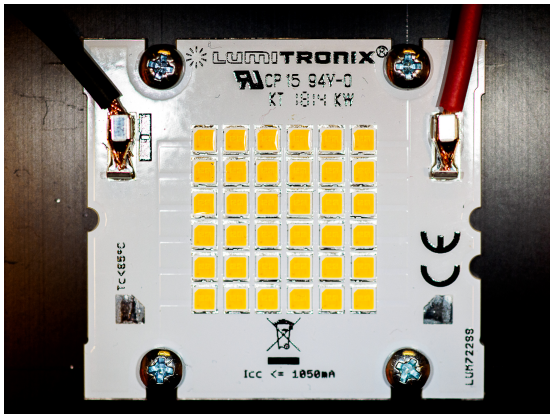


Figure 1.17: Photgraph of 'neutral white LED' array showing the yellow "phosphor" in the coating of the LEDs (Lumitronix SmartArray Q36 LED-Module, 39W, using Nichia 757 LEDs).

the beam from a 1 mW laser pointer easily visible at a distance of tens of meters in a lecture hall illuminated with lamps emitting in total hundreds of watts of visible radiation. For the same reason, even lasers emitting as little 1 mW if pointed directly into the eyes can cause permanent eye-sight damage.

2

Radiation interactions

2.1 Radiation and molecules

2.1.1 Absorption

2.1.2 Fluorescence

2.1.3 Phosphorescence

2.2 Radiation and simple objects

2.2.1 Angle of incidence

2.2.2 Refraction

2.2.3 Difraction

2.2.4 Scatering

2.3 Radiation in tissues and cells

2.4 Radiation interactions in plant canopies

The attenuation of visible and UV radiation by canopies is difficult to describe mathematically because it is a complex phenomenon. The spatial distribution of leaves is in most cases not uniform, the display angle of the leaves is not random, and may change with depth in the canopy, and even in some cases with time-of-day. Here we give only a description of the simplest approach, the use of an approximation based on Beer's law as modified by (**Monsi1953**), reviewed by (**Hirose2005**). Beer's law (Equation 1.8) assumes a homogeneous light absorbing medium such as a solution. However, a canopy is heterogenous, with discrete light absorbing objects (the leaves and stems) distributed in a transparent medium (air).

$$I_z = I_0 \cdot \mathrm{e}^{-K L_z} \tag{2.1}$$

Equation 2.1 describes the radiation attenuated as a function of leaf area index (L or LAI) at a given canopy depth (z). The equation does not explicitly account for the effects of the statistical spatial distribution of leaves and the effects of changing incidence angle of the radiation. Consequently, the empirical extinction coefficient (K) obtained may vary depending on these factors. K is not only a function of plant species (through leaf optical properties, and how leaves are displayed), but also of time-of-day, and season-of-year—as a consequence of solar zenith angle—and degree of scattering of the incident radiation. As the degree of scattering depends on clouds,

and also on wavelength, the extinction coefficient is different for UV and visible radiation. Radiation extinction in canopies has yet to be studied in detail with respect to UV radiation, mainly because of difficulties in the measurement of UV radiation compared to PAR, a spectral region which has been extensively studied.

Ultraviolet radiation is strongly absorbed by plant surfaces, although cuticular waxes and pubescence on leaves can sometimes increase UV reflectance. The diffuse component of UV radiation is larger than that of visible light (Figure **??**). In sunlit patches in forest gaps the diffuse radiation percentage is lower than in open areas, because direct radiation is not attenuated but part of the sky is occluded by the surrounding forest. Attenuation with canopy depth is on average usually more gradual for UV than for PAR. The UV irradiance decreases with depth in tree canopies, but the UV:PAR ratio tends to increase (**Brown1994**). In contrast, (**Deckmyn2001**) observed a decrease in UV:PAR ratio in white clover canopies with planophyle leaves. (**Allen1975**) modelled the UV-B penetration in plant canopies, under normal and depleted ozone conditions. (**Parisi1996**) measured UV-B doses within model plant canopies using dosimeters. The position of leaves affects UV-B exposure, and it has been observed that heliotropism can moderate exposure and could be a factor contributing to differences in tolerance among crop cultivars (**Grant1998**; **Grant1999**; **Grant1999a**; **Grant2004**).

Detailed accounts of different models describing the interaction of radiation and plant canopies, taking into account the properties of foliage, are given by (**Campbell1998**) and (**Monteith2008**).

2.5 Radiation interactions in water bodies

Missing for now…

2.6 Physical quantities

2.6.1 Specular and total reflectance

2.6.2 Internal and total transmittance

2.6.3 Absorbance and absorptance

3

Photochemistry and photobiology

Part II

Tools used for calculations

4

Software

4.1 Introduction

The software used for typesetting this handbook and developing the r4photobiology suite is free and open source. All of it is available for the most common operating systems (Unix including OS X, Linux and its variants, and Windows). It is also possible to run everything described here on a Linux server running the server version of RStudio, and access the server through a web browser.

For just running the examples in the handbook, you would need only to have R installed. That would be enough as long as you also have a text editor available. This is possible, but does not give a very smooth workflow for data analyses which are beyond the very simple. The next stage is to use a text editor which integrates to some extent with R, but still this is not ideal, specially for writing packages or long scripts. Currently the best option is to use the integrated development environment (IDE) called 'RStudio'. This is an editor, but tightly integrated with R. Its advantages are especially noticeable in the case of errors and 'debugging'. During the development of the packages, we used RStudio exclusively.

The typesetting is done with LaTeX and the source of this handbook was edited using both the shareware editor WinEdt (which excels as a LaTeX editor) and RStudio which is better suited to the debugging of the code examples. We also used LaTeX for our first handbook (**Aphalo2012**).

Combining R with Markdown (Rmarkdown: Rmd files) or LaTeX (Rnw files) to produce *literate* scripts is best for reproducible research and our suite of packages is well suited for this approach to data analysis. However, it is not required to go this far to be able to profit from R and our suite for simple analyses, but the set up we will describe here, is what we currently use, and it is by far the best one we have encountered in 18 years of using and teaching how to use R.

We will not give software installation instructions in this handbook, but will keep a web page with up-to-date instructions. In the following sections we briefly describe the different components of a full and comfortable working environment, but there are many alternatives and the only piece that you cannot replace is R itself.

4.2 The different pieces

4.2.1 R

You will not be able to profit from this handbook's 'Cook Book' part, unless you have access to R. R (also called Gnu S) is both the name of a software system, and a dialect of the language S. The language S, although designed with data analysis and statistics in mind, is a computer language that is very powerful in its own way. It allows object

oriented programming. Being based on a programming language, and being able to call and being called by programs and subroutine libraries written in several other programming languages, makes R easily extensible.

R has a well defined mechanism for "addons" called packages, that are kept in the computer where R is running, in disk folders that conform the library. There is a standard mechanism for installing packages, that works across operating systems (OSs) and computer architectures. There is also a Comprehensive R Archive Network (CRAN) where publicly released versions of packages are kept. Packages can be installed and updated from CRAN and similar repositories directly from within R.

The *engine* behind the production of the pages of this handbook is the R package 'knitr' which allows almost seamless integration of R code and text marked up using LaTeX. We have used in addition several other packages, both as building blocks in our packages, and for the production of the examples. The most notable ones are: 'tibble', 'dplyr', 'readr', 'lubridate', 'ggplot2', and 'ggtern'. Packages 'devtools' and 'testthat' significantly easied the task of package development and coding.

If you are not familiar with R, please, before continuing reading this handbook read a book on the R *language* itself—rather than a book on statistics with R. The book 'Learning R …as you learnt your mother tongue' (**Aphalo2016**) takes the approach of learning the R language through exploration, which is the way many experienced R programmers unravel the intricacies of the language. In contrast the more concise book 'R Programming for Data Science' (**Peng2015**) takes a more direct and possibly less challenging approach to teaching the R language. There is also a free introduction to R (**Paradis2005**) available at `https://cran.r-project.org/doc/contrib/Paradis-rdebuts_en.pdf` and a 'student's Guide to R' (**Horton2015**) at `https://cran.r-project.org/doc/contrib/Horton+Pruim+Kaplan_MOSAIC-StudentGuide.pdf`.

4.2.2 RStudio

RStudio is an intergrated development environment (IDE). The difference between an IDE and an editor is that an IDE integrates additional tools that facilitate the interaction with R. RStudio highlights the R code according to the syntax, offers autocompletion while typing, highlights invalid code on the fly. When a script is run, if an error is triggered, it automatically find the location of the error. RStudio also supports the concept of projects allowing saving of settings separately. It also integrates support for file version control (see next section).

RStudio exists in two versions with identical user interface: a desktop version and a server version. The server version can be used remotely through a web browser. It can be run in the 'cloud', for example, as an AWS instance (Amazon Web Services) quite easily and cheaply, or on one's own server hardware. RStudio is under active development, and constantly improved (visit `http://www.rstudio.org/` for an up-to-date description and download and installation instructions.

Two books (**vanderLoo2012**; **Hillebrand2015**) describe and teach how to use RStudio without going in depth into data analysis or statistics, however, as RStudio is under very active development new features are or will be missing from these books as time goes by. You will find tutorials and up-to-date cheat sheets at `http://www.rstudio.org/`.

4.2.3 Revision control: Git and Subversion

Revision control systems help by keeping track of the history of software development, data analysis, or even manuscript writing. They make it possible for several programmers, data analysts, authors and or editors to work on the same files in parallel and then merge their edits. They also allow easy transfer of whole 'projects' between computers. Git is very popular, and Github and Bitbucket are popular hosts for repositories. Git itself is free software, was designed by Linus Tordvals of Linux fame, and can be also run locally, or as one's own private server, either as an AWS instance or on other hosting service, or on your own hardware.

The books 'Git: Version Control for Everyone' (**Somasundaram2013**) and 'Pragmatic Guide to Git' (**Swicegood2010**) are good introductions to revision control with Git. Free introductory videos and cheatsheets are available at `https://git-scm.com/doc`.

4.2.4 C++ compiler

Although R is an interpreted language, a few functions in our suite are written in C++ to achieve better performance. On OS X and Windows, the normal practice is to install binary packages, which are ready compiled. In other systems like Linux and Unix it is the normal practice to install source packages that are compiled at the time of installation. With suitable build tools (e.g. RTools for Windows) source packages can be installed and developed in any of the operating systems on which R runs.

4.2.5 LaTeX

LaTeX is built on top of TeX. TeX code and features were 'frozen' (only bugs are fixed) long ago. There are currently a few 'improved' derivatives: pdfTeX, XeTeX, and LuaTeX. Currently the most popular TeX in western countries is pdfTeX which can directly output PDF files. XeTeX can handle text both written from left to right and right to left, even in the same document and additional font formats, and is the most popular TeX engine in China and other Asian countries. Both XeLaTeX and LuaTeX are rapidly becoming popular also for typesetting texts in variants of Latin and Greek alphabets as these new TeX engines natively support large character sets and modern font formats such as TTF (True Type) and OTF (Open Type).

For the typesetting of this handbook we used several LaTeX packages, of which those that most affected appearance are 'KOMA-script', 'hyperref', 'booktabs', 'pgf/tikz' and 'biblatex'. The TeX used is MikTeX.

4.2.6 Markdown

Markdown is a simple markup language, which although offering somehow less flexibility that LaTeX is much easier to learn and which can be easily converted to various output formats such as HTMLand XTML in addition to PDF. RStudio supports editing markdown and the variants R Markdown and Bookdown. Documentation on Rmarkdown is available on-line at `http://rmarkdown.rstudio.com/` and on Bookdown at `https://bookdown.org/`.

5

Photobiology R packages

5.1 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'.

5.2 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 5.1). 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 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 for methods as well as consistency in the order of arguments across the suite should reduce the number of *names* to remember. Data objects are *tidy* as defined by in (**Wickham2014a**), 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.

As an example, the same summary methods, are available for individual spectra (`_spct` objects) and and collections of spectra (`_mspct` objects), in the first case returning a numeric 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' of code from which specific methods can be constructed,

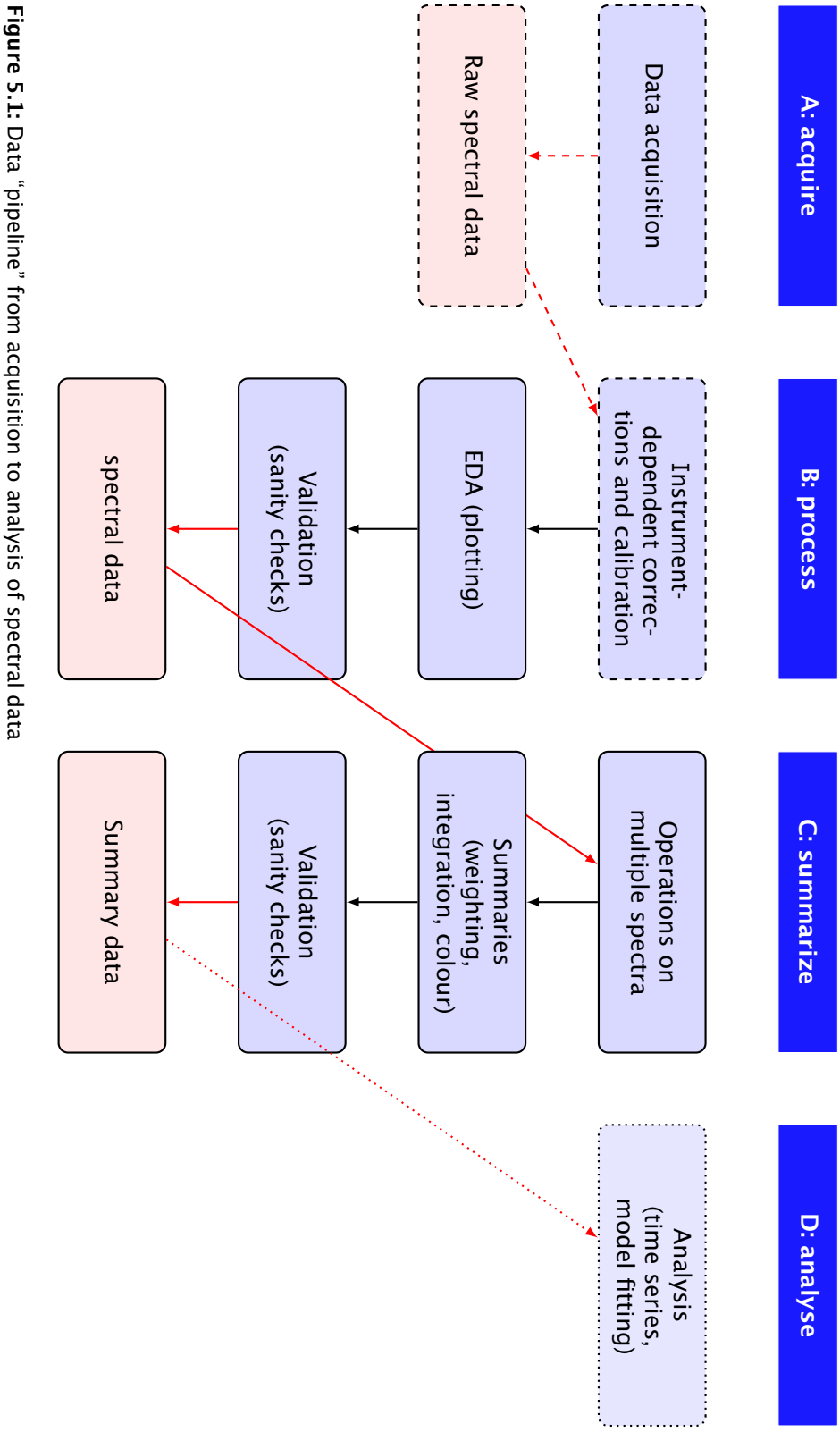


Figure 5.1: Data "pipeline" from acquisition to analysis of spectral data

Box 5.1: 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.

`_mspct` 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.

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

`apply` **methods** Used to apply functions individual spectra stored in collections of spectra.

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

`plot` **methods** Simplify the construction of specialized plots of spectral data.

foreign data exchange functions For importing data output by measuring instruments and exchanging data with other R packages.

plus ready defined methods for frequently used operations. 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 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 bottlenecks by extensive testing and in isolated cases writing functions in C++.

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

Is all what is needed to obtain the CIE98-weighted 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 automat-

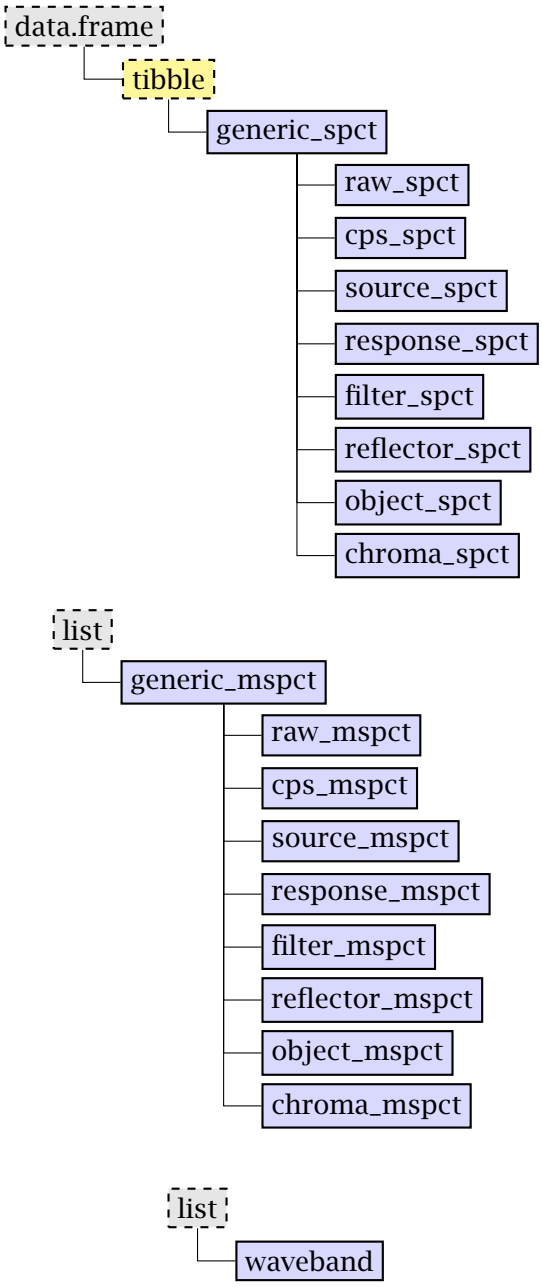


Figure 5.2: Object classes used in the packages. Objects of _spct classes are used to store spectra, in most cases a single spectrum. Objects of _mspct classes can be used to store *collections* of _spct objects, in most cases all belonging to the same class. Objects of class waveband contain information 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 CRAN, Comprehensive R Archive Network, and blue-filled boxes represent classes defined in package 'photobiology'.

Table 5.1: Packages in the r4photobiology suite. Packages not yet released are marked with a red bullet •, and those at 'beta' stage with a yellow bullet •, those relatively stable with a green bullet •, and those in CRAN with the label CRAN in the first column of the table.

	Package	Type	Contents
•	photobiologyAll	dummy	loads other packages of the suite
CRAN	photobiology	funs + classes	basic functions, class definitions, class methods and example data
CRAN	photobiologyInOut	functions	data import/export functions
CRAN	photobiologyWavebands	definitions	quantification of radiation
CRAN	ggspectra	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	driver API	Ocean Optics spectrometers
•	ooacquire	data acquistion	Ocean Optics spectrometers

ically 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.

5.3 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 5.1).

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

Wavelengths should always be in nanometres (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.

5.4 The r4photobiology repository

Four of the packages are already available through CRAN, the 'Comprehensive R Archive Network'. For distributing other packages in the suite, I have created a repository at `http://r4photobiology.info/R`. This repository follows the CRAN folder structure, so package installation can be done using normal R commands. Consequently dependencies are installed automatically and 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"))
```

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

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* (i.e. executed) 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", "ggspectra"))
```

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

6

Storing data

6.1 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)
library(photobiologyWavebands)
```

6.2 Introduction

The suite uses object-oriented programming for its higher level 'user-friendly' syntax. Objects are implemented using "S3" classes. The two main distinct kinds of objects are different types of spectra, and wavebands. Spectral objects contain, as their name implies, spectral data. Wavebands contain the information needed to calculate irradiance, non-weighted or weighted (effective), and a name and a label to be used in output printing. Functions and operators are defined for operations on these objects, alone and in combination. We will first describe spectra, and then wavebands, in each case describing operators and functions. See Chapter 5 on page 37 for a detailed description of the classes defined by the packages.

6.3 Spectra

6.3.1 How are spectra stored?

For spectra the classes are a specialization of `tibble` which are derived from `data.frame`. This means that they are compatible with functions that operate on objects of these classes. See the documentation of package 'tibble' for a description of the advantages of this class compared to base R's data frames.

The suite defines a `generic_spct` class, from which other specialized classes, ' `filter_spct`, `reflector_spct`, `object_spct`, `source_spct`, `response_spct`, `response_spct`, `chroma_spct` and `cps_spct` are derived. Having this class structure allows us to create special methods and operators, which use the same 'names' than the generic ones defined by R itself, but take into account the special properties of spectra.

In most cases each spectral object holds only spectral data from a single measurement event. When spectral data from more than one measurement is contained in a single object, the data for the different measurements are stored *lengthwise*, in

Table 6.1: Classes for spectral data and *mandatory* variable and attribute names

Name	Variables	Attributes
generic_spct	w.length	
raw_spct	w.length, counts	instr.desc, instr.settings
cps_spct	w.length, cps	instr.desc, instr.settings
source_spct	w.length, s.e.irrad, s.q.irrad	time.unit, bswf
filter_spct	w.length, Tfr, A	Tfr.type
reflector_spct	w.length, Rfr	Rfr.type
object_spct	w.length, Tfr, Rfr	Tfr.type, Rfr.type
response_spct	w.length, s.e.response, s.q.response	time.unit
chroma_spct	w.length, x, y, z	

other words, in the same variable(s), and distinguished by means of an index factor. When a single measurement consists in several different quantities being measured, then these are stored in different variables, or columns, in the same spectral object. Variables containing spectral data for a given quantity have consistent *mandatory* names, and data are always stored using the same units. Spectral objects also carry additional information in attributes, such a text 'comment', the time unit used for expression, and additional attributes indicating properties such as whether reflectance is **specular** or **total**. Optional attributes with mandatory naming are used to store metadata such as the time and geographical coordinates of a measurement in a consistent way. These strict rules allow the functions in the package to handle unit conversions, and units in labels and plots automatically. It also allows the use of operators like ('+') with spectra, and some sanity checks on the supplied spectral data and prevention of *some* invalid operations. Table 6.1 lists the mandatory names of variables and attributes for each of the classes. In Table 6.2 for each mandatory variable name, plus the additional names recognized by constructors are listed together with the respective units. Additional columns are allowed in the spectral objects, and deleted or set to `NA` only when the meaning of an operation on the whole spectrum is for these columns ambiguous. The *User Guide* of package 'photobiology' contains detailed tables of classes, operators and methods.

6.3.2 Spectral data assumptions

The packages' code assumes that wavelengths are always expressed in nanometres ($1\ \text{nm} = 1 \cdot 10^{-9}$ m). If the data to be analysed uses different units for wavelengths, e.g. Ångstrom ($1\ \text{Å} = 1 \cdot 10^{-10}$ m), the values need to be re-scaled before any calculations. The assumptions related to the expression of spectral data should be followed strictly as otherwise the results returned by calculations will be erroneous. Table 6.2 lists the units of expression for the different variables listed in Table 6.1. Object constructors accept, if properly instructed, spectral data expressed in some cases differently than the format used for storage. In such cases unit conversion during object creation is automatic. For example, although transmittance is always stored as a fraction of one in variable `Tfr`, the constructors recognize variable `Tpc` as expressed as a percent and convert the data and rename the variable.

The attributes related to the stored quantities add additional flexibility, and are

Table 6.2: Variables used for spectral data and their units of expression: A: as stored in objects of the spectral classes, B: also recognized by the `set` family of functions for spectra and automatically converted. `time.unit` accepts in addition to the character strings listed in the table, objects of classes `lubridate::duration` and `period`, in addition `numeric` values are interpreted as seconds. `exposure.time` accepts these same values, but not the character strings.

Variables	Unit of expression	Attribute value
A: stored		
w.length	nm	
counts	number	
cps	$n\,s^{-1}$	
s.e.irrad	$W\,m^{-2}\,nm^{-1}$	time.unit = "second"
s.e.irrad	$J\,m^{-2}\,d^{-1}\,nm^{-1}$	time.unit = "day"
s.e.irrad	varies	time.unit = *duration*
s.q.irrad	$mol\,m^{-2}\,s^{-1}\,nm^{-1}$	time.unit = "second"
s.q.irrad	$mol\,m^{-2}\,d^{-1}\,nm^{-1}$	time.unit = "day"
s.q.irrad	$mol\,m^{-2}\,nm^{-1}$	time.unit = "exposure"
s.q.irrad	varies	time.unit = *duration*
Tfr	[0,1]	Tfr.type = "total"
Tfr	[0,1]	Tfr.type = "internal"
A	a.u.	Tfr.type = "internal"
Rfr	[0,1]	Rfr.type = "total"
Rfr	[0,1]	Rfr.type = "specular"
s.e.response	$x\,J^{-1}\,s^{-1}\,nm^{-1}$	time.unit = "second"
s.e.response	$x\,J^{-1}\,d^{-1}\,nm^{-1}$	time.unit = "day"
s.e.response	$x\,J^{-1}\,nm^{-1}$	time.unit = "exposure"
s.e.response	varies	time.unit = *duration*
s.q.response	$x\,mol^{-1}\,s^{-1}\,nm^{-1}$	time.unit = "second"
s.q.response	$x\,mol^{-1}\,d^{-1}\,nm^{-1}$	time.unit = "day"
s.q.response	$x\,mol^{-1}\,nm^{-1}$	time.unit = "exposure"
s.q.response	varies	time.unit = *duration*
x, y, z	[0,1]	
B: converted		
wl → w.length	nm	
wavelength → w.length	nm	
Tpc → Tfr	[0,100]	Tfr.type = "total"
Tpc → Tfr	[0,100]	Tfr.type = "internal"
Rpc → Rfr	[0,100]	Rfr.type = "total"
Rpc → Rfr	[0,100]	Rfr.type = "specular"
counts.per.second → cps	$n\,s^{-1}$	

normally set when an object spectral object is created, either to a default or a value supplied by the user. Attribute values can be also retrieved and set from existing objects.

 Not respecting data assumptions will yield completely wrong results! It is extremely important to make sure that the wavelengths are in nanometres as this is what all functions expect. If wavelength values are in the wrong units, the action-spectra weights and quantum conversions will be wrongly calculated, and the values returned by most functions completely wrong, without warning. The assumptions related to spectral data need also to be strictly followed, as the packages do automatically use the assumed units of expression when printing and plotting results.

6.3.3 Task: Create a spectral object from numeric vectors

'Traditional' constructor functions are available, and possibly easiest to use to those used R programming style. Constructor functions have the same name as the classes (e.g. `source_spct`). The constructor functions accept numeric vectors as arguments, and these can be "renamed" on the fly. The object is checked for consistency and within-range data, and missing required components are set to `NA`. We use `source_spct` in the examples but similar functions are defined for all the classes spectral objects.

We can create a new object of class `source_spct` from two `numeric` vectors, and as shown below, recycling applies.

```
source_spct(w.length = 300:500, s.e.irrad = 1)

## Object: source_spct [201 x 2]
## Wavelength range 300 to 500 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 201 x 2
##   w.length s.e.irrad
##      <int>     <dbl>
## 1      300         1
## 2      301         1
## 3      302         1
## 4      303         1
## 5      304         1
## # ... with 196 more rows
```

The code above uses defaults for all attributes, and assumes that spectral energy irradiance is expressed in $\mathrm{W\,m^{-2}\,nm^{-1}}$. As elsewhere in the package, wavelengths should be expressed in nanometres. If our spectral data is in photon-based units with spectral photon irradiance expressed in $\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$ the code becomes:

```
source_spct(w.length = 300:500, s.q.irrad = 1)

## Object: source_spct [201 x 2]
## Wavelength range 300 to 500 nm, step 1 nm
```

```
## Time unit 1s
##
## # A tibble: 201 x 2
##   w.length s.q.irrad
##      <int>     <dbl>
## 1      300         1
## 2      301         1
## 3      302         1
## 4      303         1
## 5      304         1
## # ... with 196 more rows
```

Spectral objects have attributes, which store additional information needed for correct handling of units of expression, printing and plotting. The defaults need frequently to be changed, for example when spectral exposure is expressed as a daily integral, or other arbitrary exposure time. This length of time or `duration` should be set, whenever the unit of time used is different to second.

```
source_spct(w.length = 300:500, s.q.irrad = 1, time.unit = "day")

## Object: source_spct [201 x 2]
## Wavelength range 300 to 500 nm, step 1 nm
## Time unit 86400s (~1 days)
##
## # A tibble: 201 x 2
##   w.length s.q.irrad
##      <int>     <dbl>
## 1      300         1
## 2      301         1
## 3      302         1
## 4      303         1
## 5      304         1
## # ... with 196 more rows
```

In addition to the character strings `"second"`, `"hour"`, and `"day"`, any object belonging to the class `duration` defined in package 'lubridate' can be used. This means, that any arbitrary time duration can be used.

Please, see Tables 6.1 and 6.2 for the attributes defined for the different classes of spectral objects.

Task: Manual unit conversion

If spectral irradiance data is in $\mathrm{W\,m^{-2}\,nm^{-1}}$, and the wavelength in nm, as is the case for many Macam spectroradiometers, the data can be used directly and functions in the package will return irradiances in $\mathrm{W\,m^{-2}}$.

If, for example, the spectral irradiance data output by a spectroradiometer is expressed in $\mathrm{mW\,cm^{-2}\,nm^{-1}}$, and the wavelengths are in Ångstrom then to obtain correct results when using any of the packages in the suite, we need to rescale the data before creating a new object.

```
# not run
my.spct <-
   source_spct(w.length = wavelength / 10, s.e.irrad = irrad / 1000)
```

In the example above, we take advantage of the behaviour of the S language: an operation between a scalar and vector, is equivalent to applying this operation to each member of the vector. Consequently, in the code above, each value from the vector of wavelengths is divided by 10, and each value in the vector of spectral irradiance is divided by 1000.

6.3.4 Task: Create a spectral object from a data frame

'Traditional' conversion functions with names given by names of classes preceded by `as.` (e.g. `as.source_spct`. These functions accept data frames, data tables, and lists with components of equal length as arguments. These functions are less flexible, as the component variables in the argument should be named using one of the names recognized. Table **??** lists the different 'names' understood by these constructor functions and the required and optional components of the different spectral object classes. The object is checked for consistency and within-range data, and missing required components are set to `NA`. We use `source_spct` in the examples but similar functions are defined for all the classes spectral objects.

We first use a `data.frame` containing suitable spectral data. Object `sun.data` is included as part of package 'photobiology'. Using `head` we can check that the names of the variables are the expected ones, and that the wavelength values are expressed in nanometres:

```
#is.data.frame(sun.data)
#head(sun.data, 3)
```

Subsequently we create a new `source_spct` object by copy:

```
first.sun.spct <- as.source_spct(sun.data)
is.source_spct(first.sun.spct)

## [1] TRUE
```

In this case `sun.data` remains independent, and whatever change we make to `my.sun.spct` does not affect `sun.data`. The `as.` functions, first make a copy of the data frame or data table, and then call one of the `set` functions described in section the section to convert the copy into a `_spct` object. Table **??** lists the different 'names' understood by these copy functions and the required and optional components of the different spectral object classes. The new object is checked for consistency and within-range data, and missing required components are set to `NA`. We use `source_spct` in the examples but similar functions are defined for all the classes spectral objects. In the same way as constructors, the `as.` functions accept attributes such as `time.unit` as arguments.

Using a technical term, `as.` functions are *copy constructors*, which follow the *normal* behaviour of the R language.

6.3.5 Task: Convert a data frame into a spectral object

The last possibility, is to use a syntax that is unusual for the R language, but which in some settings will lead to faster execution: convert an existing data frame, *in situ*

or by reference, into a `source_spct` object. The `set` functions defined in package 'photobiology' have the same semantics as `setDT` and `setDF` from package `data.table`. Table ?? lists the different 'names' understood by these conversion functions and the required and optional components of the different spectral object classes. The object is checked for consistency and within-range data, and missing required components are set to `NA`. We use `source_spct` in the examples but similar functions are defined for all the classes spectral objects. In the same way as constructors, the `set` functions accept attributes such as `time.unit` as arguments.

```
second.sun.spct <- sun.data
setSourceSpct(second.sun.spct)
is.source_spct(second.sun.spct)

## [1] TRUE
```

We normally do not use the value returned by `set` functions as it is just a reference the original object, and assigning this value to another name will result in two names pointing to the same object.

In fact, the assignment is unnecessary, as the class of `my.df` is set:

```
third.sun.spct <- sun.data
fourth.sun.spct <- setSourceSpct(second.sun.spct)
third.sun.spct

## # A tibble: 508 x 3
##   w.length    s.e.irrad    s.q.irrad
##       <dbl>        <dbl>        <dbl>
## 1      293 2.609665e-06 6.391730e-12
## 2      294 6.142401e-06 1.509564e-11
## 3      295 2.176175e-05 5.366385e-11
## 4      296 6.780119e-05 1.677626e-10
## 5      297 1.533491e-04 3.807181e-10
## # ... with 503 more rows

fourth.sun.spct$s.e.irrad <- NA
third.sun.spct

## # A tibble: 508 x 3
##   w.length    s.e.irrad    s.q.irrad
##       <dbl>        <dbl>        <dbl>
## 1      293 2.609665e-06 6.391730e-12
## 2      294 6.142401e-06 1.509564e-11
## 3      295 2.176175e-05 5.366385e-11
## 4      296 6.780119e-05 1.677626e-10
## 5      297 1.533491e-04 3.807181e-10
## # ... with 503 more rows
```

Using a technical term, `set` functions convert an object by *reference*, which is *not* the normal behaviour in the R language.[1]

[1] Avoiding copying can improve performance for huge objects, but will rarely make a tangible difference for individual spectra of moderate size.

6.3.6 Task: trimming a spectrum

This is basically a subsetting operation, but our functions operate only based on wavelengths, while R `subset` is more general. On the other hand, our functions `trim_spct` and `trim_tails` add a few 'bells and whistles'. The trimming is based on wavelengths and by default the cut points are inserted by interpolation, so that the spectrum returned includes the limits given as arguments. In addition, by default the trimming is done by deleting both spectral irradiance and wavelength values outside the range delimited by the limits (just like `subset` does), but through parameter `fill` the values outside the limits can be replaced by any value desired (most commonly `NA` or 0.) It is possible to supply a only one, or both of `low.limit` and `high.limit`, depending on the desired trimming, or use a `waveband` definition or a numeric vector as an argument for `range`. If the limits are outside the original data set, then the output spectrum is expanded and the tails filled with the value given as argument for `fill` unless `fill` is equal to `NA`, which is the default.

```
trim_wl(sun.spct, range = UV())

## Object: source_spct [122 x 3]
## Wavelength range 280 to 400 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 122 x 3
##   w.length s.e.irrad s.q.irrad
## *    <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## 5 283.6923         0         0
## # ... with 117 more rows

trim_wl(sun.spct, range = UV(), fill = 0)

## Object: source_spct [705 x 3]
## Wavelength range 100 to 800 nm, step 1.023182e-12 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 705 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 100.0000         0         0
## 2 100.9945         0         0
## 3 101.9890         0         0
## 4 102.9834         0         0
## 5 103.9779         0         0
## # ... with 700 more rows

trim_wl(sun.spct, range = c(400, NA))

## Object: source_spct [401 x 3]
## Wavelength range 400 to 800 nm, step 1 nm
## Measured on 2010-06-22 09:51:00 UTC
```

```
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 401 x 3
##   w.length s.e.irrad    s.q.irrad
## *    <dbl>     <dbl>        <dbl>
## 1      400 0.6081049 2.033314e-06
## 2      401 0.6261742 2.098967e-06
## 3      402 0.6497388 2.183388e-06
## 4      403 0.6207287 2.091091e-06
## 5      404 0.6370489 2.151395e-06
## # ... with 396 more rows
```

```
trim_wl(sun.spct, range = c(250, NA), fill = 0.0)
```

```
## Object: source_spct [554 x 3]
## Wavelength range 250 to 800 nm, step 1.023182e-12 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 554 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 250.0000         0         0
## 2 250.9677         0         0
## 3 251.9355         0         0
## 4 252.9032         0         0
## 5 253.8710         0         0
## # ... with 549 more rows
```

```
trim_wl(sun.spct, range = c(300, 400, 500, 600))
```

```
## Object: source_spct [301 x 3]
## Wavelength range 300 to 600 nm, step 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 301 x 3
##   w.length   s.e.irrad    s.q.irrad
## *    <dbl>       <dbl>        <dbl>
## 1      300 0.001264554 3.171207e-09
## 2      301 0.002623718 6.601607e-09
## 3      302 0.003922583 9.902505e-09
## 4      303 0.008974134 2.273009e-08
## 5      304 0.011655666 2.961943e-08
## # ... with 296 more rows
```

If the limits are outside the range of the input spectral data, and `fill` is set to a value other than `NULL` the output is expanded up to the limits and filled.

```
trim_wl(sun.spct, range=c(300, 1000))
```

```
## Object: source_spct [501 x 3]
## Wavelength range 300 to 800 nm, step 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
```

```
## # A tibble: 501 x 3
##   w.length   s.e.irrad    s.q.irrad
## *    <dbl>       <dbl>        <dbl>
## 1      300 0.001264554 3.171207e-09
## 2      301 0.002623718 6.601607e-09
## 3      302 0.003922583 9.902505e-09
## 4      303 0.008974134 2.273009e-08
## 5      304 0.011655666 2.961943e-08
## # ... with 496 more rows

trim_wl(sun.spct, range=c(300, 1000), fill = NA)

## Object: source_spct [725 x 3]
## Wavelength range 280 to 1000 nm, step 1.023182e-12 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 725 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 280.0000        NA        NA
## 2 280.9231        NA        NA
## 3 281.8462        NA        NA
## 4 282.7692        NA        NA
## 5 283.6923        NA        NA
## # ... with 720 more rows

trim_wl(sun.spct, range=c(300, 1000), fill = 0.0)

## Object: source_spct [725 x 3]
## Wavelength range 280 to 1000 nm, step 1.023182e-12 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 725 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## 5 283.6923         0         0
## # ... with 720 more rows
```

Function `trim_tails` can be used for trimming spectra when data is available as vectors.

6.3.7 Task: interpolating a spectrum

Functions `interpolate_spct` and `interpolate_spectrum` allow interpolation to different wavelength values. `interpolate_spectrum` is used internally, and accepts spectral data measured at arbitrary wavelengths. Raw data from array spectrometers is not available with a constant wavelength step. It is always best to do any interpolation as late as possible in the data analysis.

In this example we generate interpolated data for the range 280 nm to 300 nm at

1 nm steps, by default output values outside the wavelength range of the input are set to `NA`s unless a different argument is provided for parameter `fill`:

```
interpolate_spct(sun.spct, seq(290, 300, by=0.1))

## Object: source_spct [101 x 3]
## Wavelength range 290 to 300 nm, step 0.1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 101 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1    290.0         0         0
## 2    290.1         0         0
## 3    290.2         0         0
## 4    290.3         0         0
## 5    290.4         0         0
## # ... with 96 more rows

interpolate_spct(sun.spct, seq(290, 300, by=0.1), fill=0.0)

## Object: source_spct [101 x 3]
## Wavelength range 290 to 300 nm, step 0.1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 101 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1    290.0         0         0
## 2    290.1         0         0
## 3    290.2         0         0
## 4    290.3         0         0
## 5    290.4         0         0
## # ... with 96 more rows
```

`interpolate_spct` accepts any spectral object, and returns an object of the same type as its input.

```
interpolate_spct(polyester.spct, seq(290, 300, by=0.1))

## Object: filter_spct [101 x 2]
## Wavelength range 290 to 300 nm, step 0.1 nm
##
## # A tibble: 101 x 2
##   w.length   Tfr
##      <dbl> <dbl>
## 1    290.0 0.004
## 2    290.1 0.004
## 3    290.2 0.004
## 4    290.3 0.004
## 5    290.4 0.004
## # ... with 96 more rows
```

Function `interpolate_spectrum` takes numeric vectors as arguments, but is otherwise functionally equivalent.

These functions, in their current implementation, always return interpolated values, even when the density of wavelengths in the output is less than that in the input. A future version of the package will include a `smooth_spectrum` function, and possibly a `remap_w.length` function that will automatically choose between interpolation and smoothing/averaging as needed.

6.3.8 Task: Row binding spectra

Sometimes, especially for plotting, we may want to row-bind spectra. When the aim is that the returned object retains its class attributes, and other spectrum related attributes like the time unit, functions `rbind` from base R, should NOT be used. Package 'photobiology' provides function `rbinspct` for row-binding spectra, with the necessary checks for consistency of the bound spectra.

```
# STOPGAP
shade.spct <- sun.spct
```

```
rbindspct(list(sun.spct, shade.spct))
```

```
## Object: source_spct [1,044 x 4]
## containing 2 spectra in long form
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Time unit 1s
##
## # A tibble: 1,044 x 4
##   w.length s.e.irrad spct.idx s.q.irrad
##      <dbl>     <dbl>   <fctr>     <dbl>
## 1 280.0000         0   spct_1         0
## 2 280.9231         0   spct_1         0
## 3 281.8462         0   spct_1         0
## 4 282.7692         0   spct_1         0
## 5 283.6923         0   spct_1         0
## # ... with 1,039 more rows
```

It is also possible to add an ID factor, to be able to still recognize the origin of the observations after the binding. If the supplied list is anonymous, then capital letters will be used for levels.

```
rbindspct(list(sun.spct, shade.spct), idfactor = TRUE)
```

```
## Object: source_spct [1,044 x 4]
## containing 2 spectra in long form
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Time unit 1s
##
## # A tibble: 1,044 x 4
##   w.length s.e.irrad spct.idx s.q.irrad
##      <dbl>     <dbl>   <fctr>     <dbl>
## 1 280.0000         0   spct_1         0
## 2 280.9231         0   spct_1         0
## 3 281.8462         0   spct_1         0
## 4 282.7692         0   spct_1         0
```

```
## 5 283.6923         0   spct_1         0
## # ... with 1,039 more rows
```


In contrast, if a named list with no missing names, is supplied as argument, these names are used for the levels of the ID factor.

```
rbindspct(list(sun = sun.spct, shade = shade.spct), idfactor = TRUE)

## Object: source_spct [1,044 x 4]
## containing 2 spectra in long form
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Time unit 1s
##
## # A tibble: 1,044 x 4
##   w.length s.e.irrad spct.idx s.q.irrad
##      <dbl>     <dbl>   <fctr>     <dbl>
## 1 280.0000         0      sun         0
## 2 280.9231         0      sun         0
## 3 281.8462         0      sun         0
## 4 282.7692         0      sun         0
## 5 283.6923         0      sun         0
## # ... with 1,039 more rows
```

If a character string is supplied as argument, then this will be used as the name of the factor.

```
rbindspct(list(sun = sun.spct, shade = shade.spct), idfactor = "ID")

## Object: source_spct [1,044 x 4]
## containing 2 spectra in long form
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Time unit 1s
##
## # A tibble: 1,044 x 4
##   w.length s.e.irrad     ID s.q.irrad
##      <dbl>     <dbl> <fctr>     <dbl>
## 1 280.0000         0    sun         0
## 2 280.9231         0    sun         0
## 3 281.8462         0    sun         0
## 4 282.7692         0    sun         0
## 5 283.6923         0    sun         0
## # ... with 1,039 more rows
```

6.3.9 Task: Merging spectra

Merging consists in merging different *columns* from two spectra into a new combined spectrum. Another name for this type of operations, as used in package 'dplyr', is 'join'. No wavelength interpolation is carried out, the two spectra must share wavelength values.

6.4 Collections of multiple spectra

6.4.1 Task: Constructing `_mspct` objects

6.4.2 Task: Retrieving `_spct` objects from `_mspct` objects

6.4.3 Task: Subsetting `_mspct` objects

6.5 Internal-use functions

The generic function `check` can be used on `generic_spct` objects (i.e. any spectral object), and depending on their class it checks that the required components are present, and in some cases whether they are within the expected range. If they are missing they are added. If it is possible to calculate the missing values from other optional components, they are calculated, otherwise they are filled with `NA`. It is used internally during the creation of spectral objects.

The function `check_spectrum` may need to be called by the user if he/she disables automatic sanity checking to increase calculation speed.

The function `insert_hinges` is used internally to insert individual interpolated values to the spectra when needed to reduce errors in calculations.

6.6 Wavebands

6.6.1 How are wavebands stored?

Wavebands are derived from R lists. All valid R operations for lists can be also used with `waveband` objects. However, there are `waveband` -specific specializations of some generic R methods as described in Chapter 7 and Chapter 9.

6.6.2 Task: Create waveband objects

Wavebands are created by means of function `waveband` which have in addition to the parameter(s) giving the wavelength range, additional arguments with default values.

The simplest `waveband` creation call is one supplying as argument just any R object for which the `range` function returns the wavelength limits of the desired band in nanometres. Such a call yields a `waveband` object defining an un-weighted range of wavelengths.

Any numeric vector of at least two elements, any spectral object or any existing `waveband` object for which a `range` method exists is valid input, as long as the values can be interpreted as wavelengths in nanometres.

```
waveband(c(300, 400))

## range.300.400
## low (nm) 300
## high (nm) 400
## weighted none

waveband(sun.spct)
```

```
## Total
## low (nm) 280
## high (nm) 800
## weighted none

waveband(c(400, 300))

## range.300.400
## low (nm) 300
## high (nm) 400
## weighted none
```

As you can see above, a name and label are created automatically for the new `waveband`. The user can also supply these as arguments, but must be careful not to duplicate existing names[2].

```
waveband(c(300, 400), wb.name="a.name")

## a.name
## low (nm) 300
## high (nm) 400
## weighted none
```

```
waveband(c(300, 400), wb.name="a.name", wb.label="A nice name")

## a.name
## low (nm) 300
## high (nm) 400
## weighted none
```

See chapter 10 on page 99, in particular sections 10.4, 10.3, and 10.5 for further examples, and a more in-depth discussion of the creation and use of *un-weighted* `waveband` objects.

For both functions, even if we supply a *weighting function* (SWF), a lot of flexibility remains. One can supply either a function that takes energy irradiance as input or a function that takes photon irradiance as input. Unless both are supplied, the missing function will be automatically created. There are also arguments related to normalization, both of the output, and of the SWF supplied as argument. In the examples above, 'hinges' are created automatically for the range extremes. When using SWF with discontinuous derivatives, best results are obtained by explicitly supplying the hinges to be used as an argument to the `waveband` call. An example follows for the definition of a waveband for the CIE98 SWF—the function `CIE_e_fun` is defined in package 'photobiologyWavebands' but any R function taking a numeric vector of wavelengths as input and returning a numeric vector of the same length containing weights can be used.

```
waveband(c(250, 400),
         weight="SWF", SWF.e.fun=CIE_e_fun, SWF.norm=298,
         norm=298, hinges=c(249.99, 250, 298, 328, 399.99, 400),
         wb.name="CIE98.298", wb.label="CIE98")
```

[2]It is preferable that `wb.name` complies with the requirements for R object names and file names, while labels have fewer restrictions as they are meant to be used only as text labels when printing and plotting.

```
## CIE98.298
## low (nm) 250
## high (nm) 400
## weighted SWF
## normalized at 298 nm
```

See chapter 11 on page 119, in particular sections **??**, **??**, and **??** for further examples, and a more in-depth discussion of the creation and use of *weighted* `waveband` objects.

6.6.3 Task: trimming a waveband

This operation either changes the boundaries of `waveband` objects, or deletes `waveband` objects from a list of waveband. The first argument can be either a `waveband` object or a list of `waveband` objects. Those wavebands fully outside the limits are always discarded and those fully within the limits always kept. In the case of those wavebands crossing a limit, if the argument `trim` is set to `FALSE`, they are discarded, but if `trim` is set to `TRUE` their boundary is moved to be at the trimming limit. Trimming is based on wavelengths and by default the cut points are inserted. Trimming is done by shrinking the waveband, expansion is not possible. During trimming labels stored in the `waveband` object are 'edited' to reflect the altered boundaries. Trimming does not affect weighting functions stored within the waveband.

```
trim_wl(UV(), range = UVB())

## UV.ISO.tr.lo.hi
## low (nm) 280
## high (nm) 315
## weighted none

trim_wl(VIS_bands(), low.limit = 400, trim = FALSE)

## [[1]]
## Purple.ISO
## low (nm) 360
## high (nm) 450
## weighted none
##
## [[2]]
## Blue.ISO
## low (nm) 450
## high (nm) 500
## weighted none
##
## [[3]]
## Green.ISO
## low (nm) 500
## high (nm) 570
## weighted none
##
## [[4]]
## Yellow.ISO
## low (nm) 570
## high (nm) 591
## weighted none
##
## [[5]]
```

```
## Orange.ISO
## low (nm) 591
## high (nm) 610
## weighted none
##
## [[6]]
## Red.ISO
## low (nm) 610
## high (nm) 760
## weighted none
```

```
trim_wl(VIS_bands(), low.limit = 400, trim = TRUE)
```

```
## [[1]]
## Purple.ISO
## low (nm) 360
## high (nm) 450
## weighted none
##
## [[2]]
## Blue.ISO
## low (nm) 450
## high (nm) 500
## weighted none
##
## [[3]]
## Green.ISO
## low (nm) 500
## high (nm) 570
## weighted none
##
## [[4]]
## Yellow.ISO
## low (nm) 570
## high (nm) 591
## weighted none
##
## [[5]]
## Orange.ISO
## low (nm) 591
## high (nm) 610
## weighted none
##
## [[6]]
## Red.ISO
## low (nm) 610
## high (nm) 760
## weighted none
```

```
trim_wl(VIS_bands(), range = c(500, 600))
```

```
## [[1]]
## Green.ISO
## low (nm) 500
## high (nm) 570
## weighted none
##
## [[2]]
## Yellow.ISO
## low (nm) 570
## high (nm) 591
```

```
## weighted none
##
## [[3]]
## Orange.ISO.tr.hi
## low (nm) 591
## high (nm) 600
## weighted none
```

```
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

7

Math operators and functions

7.1 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)
library(photobiologyWavebands)
library(photobiologyFilters)
```

7.2 Introduction

The suite uses object-oriented programming for its higher level 'user-friendly' syntax. Objects are implemented using "S3" classes. The two main distinct kinds of objects are different types of spectra, and wavebands. Spectral objects contain, as their name implies, spectral data. Wavebands contain the information needed to calculate summaries integrating a range of wavelengths, or for convoluting spectral data with a weighting function. In this chapter we do not describe functions for calculating such summaries, but instead we describe the use of the usual math operators and functions with spectra and wavebands.

7.3 Operators and operations between two spectra

All operations with spectral objects affect only the required components listed in Table 7.1, redundant components are always deleted[1], while unrecognized components, including all factors and character variables, are preserved only when one of the operands is a numeric vector of any length. There will be seldom need to add numerical components to spectral objects, and the user should take into account that the paradigm of the suite is that data from each spectral measurement is stored as a separate object. However, it is allowed, and possibly useful to have factors as components with levels identifying different bands, or color vectors with RGB values. Such ancillary information is useful for presentation and plotting and can be added with functions described in Chapter **??**. Exceptionally, objects can contain spectral data from several measurements and an additional factor indexing them. Such objects cannot be directly used with operators and summary functions, but can be a convenient format for storing related spectra.

[1] e.g. equivalent quantities expressed in different types of units, such as spectral energy irradiance and spectral photon irradiance

Table 7.1: Binary operators and operands. Validity and class of result. All operations marked 'Y' are allowed, those marked 'N' are forbidden and return `NA` and issue a warning.

e1	+	−	*	/	^	e2	result
cps_spct	Y	Y	Y	Y	Y	cps_spct	cps_spct
source_spct	Y	Y	Y	Y	Y	source_spct	source_spct
filter_spct (T)	N	N	Y	Y	N	filter_spct	filter_spct
filter_spct (A)	Y	Y	N	N	N	filter_spct	filter_spct
reflector_spct	N	N	Y	Y	N	reflector_spct	reflector_spct
object_spct	N	N	N	N	N	object_spct	–
response_spct	Y	Y	Y	Y	N	response_spct	response_spct
chroma_spct	Y	Y	Y	Y	Y	chroma_spct	chroma_spct
cps_spct	Y	Y	Y	Y	Y	numeric	cps_spct
source_spct	Y	Y	Y	Y	Y	numeric	source_spct
filter_spct	Y	Y	Y	Y	Y	numeric	filter_spct
reflector_spct	Y	Y	Y	Y	Y	numeric	reflector_spct
object_spct	N	N	N	N	N	numeric	–
response_spct	Y	Y	Y	Y	Y	numeric	response_spct
chroma_spct	Y	Y	Y	Y	Y	numeric	chroma_spct
source_spct	N	N	Y	Y	N	response_spct	response_spct
source_spct	N	N	Y	Y	N	filter_spct (T)	source_spct
source_spct	N	N	Y	Y	N	filter_spct (A)	source_spct
source_spct	N	N	Y	Y	N	reflector_spct	source_spct
source_spct	N	N	N	N	N	object_spct	–
source_spct	N	N	Y	N	N	waveband (no BSWF)	source_spct
source_spct	N	N	Y	N	N	waveband (BSWF)	source_spct

Binary maths operators (+, −, *, /), and unary math operators (+, −) are defined for spectral objects as well functions (`log`, `log10`,`sqrt`). Using operators is an easy and familiar way of doing calculations, but operators are rather inflexible (they can take at most two arguments, the operands) and performance is usually slower than with functions with additional parameters that allow optimizing the algorithm. Which operations are legal between different combinations of operands depends on the laws of Physics, but in cases in which exceptions might exist, they are allowed. This means that some mistakes can be prevented, but other may happen either with a warning or silently. So, although a class system provides a safer environment for calculations, it is not able to detect all possible 'nonsensical' calculations. The user must be aware that sanity checks and good understanding of the algorithms are still a prerequisite for reliable results.

Table **??** list the available operators and the operands accepted as legal, together with the class of the objects returned. Only in extreme cases errors will be triggered, in most cases when errors occur an operation between two `reflector_spct` yields a `reflector_spct` object, and operations between a `filter_spct` object and a `source_spct`, between a `reflector_spct` and a `source_spct`, or between two `source_spct` objects yield `source_spct` objects. The object returned contains data

only for the overlapping region of wavelengths. The objects do NOT need to have values at the same wavelengths, as interpolation is handled transparently. All four basic maths operations are supported with any combination of spectra, and the user is responsible for deciding which calculations make sense and which not. Operations can be concatenated and combined. The unary negation operator is also implemented.

We can convolute the emission spectrum of a light source and the transmittance spectrum of a filter by simply multiplying them.

```
sun.spct * polyester.spct
```

```
## Object: source_spct [533 x 2]
## Wavelength range 280 to 800 nm, step 0.07692308 to 1 nm
## Time unit 1s
##
## # A tibble: 533 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.0000         0
## 4 281.8462         0
## 5 282.0000         0
## # ... with 528 more rows
```

7.4 Operators and operations between a spectrum and a numeric vector

The same four basic math operators plus power ('^') are defined for operations between a spectrum and a numeric vector, possibly of length one. Recycling rules apply for the numeric vector. Normal R type conversions also take place, so a logical vector can substitute for a numeric one´. These operations do not alter `w.length`, just the other *required* components such as spectral irradiance and transmittance. The optional components are deleted as they can be recalculated if needed. Unrecognized 'user' components are left unchanged.

For example we can divide a spectrum by a numeric value (a vector of length 1, which gets recycle). The value returned is a spectral object of the same type as the spectral argument.

```
sun.spct / 2
```

```
## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
```

```
## 5 283.6923         0
## # ... with 517 more rows

2 * sun.spct

## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 517 more rows

sun.spct * 2

## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 517 more rows
```

7.5 Math functions taking a spectrum as argument

Logarithms (`log, log10`), square root (`sqrt`) and exponentiation (`exp`) are defined for spectra. These functions are not applied on `w.length` , but instead to the other mandatory component `s.e.irrad` , `Rfr` or `Tfr` . Any optional numeric components are discarded. Other user-supplied components remain unchanged.

```
log10(sun.spct)

## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
```

```
##      <dbl>     <dbl>
## 1 280.0000      -Inf
## 2 280.9231      -Inf
## 3 281.8462      -Inf
## 4 282.7692      -Inf
## 5 283.6923      -Inf
## # ... with 517 more rows
```


7.6 Task: Simulating spectral irradiance under a filter

Package 'photobiologyFilters' makes available many different filter spectra, from which we choose Schott filter GG400. Package 'photobiology' makes available one example solar spectrum. Using these data we will simulate the filtered solar spectrum.

```
sun.spct * schott.mspct$GG400
```

```
## Object: source_spct [533 x 2]
## Wavelength range 280 to 800 nm, step 0.07692308 to 1 nm
## Time unit 1s
##
## # A tibble: 533 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.0000         0
## 4 281.8462         0
## 5 282.0000         0
## # ... with 528 more rows
```

The GG440 data is for internal transmittance, consequently the results above would be close to the truth only for filters treated with an anti-reflection multicoating. Let's assume a filter with 9% reflectance across all wavelengths (a coarse approximation for uncoated glass):

```
sun.spct * schott.mspct$GG400 * (100 - 9) / 100
```

```
## Object: source_spct [533 x 2]
## Wavelength range 280 to 800 nm, step 0.07692308 to 1 nm
## Time unit 1s
##
## # A tibble: 533 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.0000         0
## 4 281.8462         0
## 5 282.0000         0
## # ... with 528 more rows
```

Calculations related to filters will be explained in detail in chapter 23. This is just an example of how the operators work, even when, as in this example, the wavelength values do not coincide between the two spectra.

7.7 Task: Uniform scaling of a spectrum

As noted above operators are available for `generic_spct`, `source_spct`, `filter_spct` and `reflector_spct` objects, and 'recycling' takes place when needed:

```
sun.spct

## Object: source_spct [522 x 3]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## 5 283.6923         0         0
## # ... with 517 more rows

sun.spct * 2

## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 517 more rows
```

All four basic binary operators (`+`, `-`, `*`, `/`) can be used in the same way. By default all calculations are done using energy based units, and only values in these units returned. If the operands need conversion, they are silently converted before applying the operator. The default behaviour can be switched into doing operations and returning values in photon-based units by setting an R option, using the normal R `options` mechanism.

7.7.1 Task: Arithmetic operations within one spectrum

As spectral objects behave in many respects as data frames it is possible to do calculations involving columns as usual, e.g. using `with` or explicit selectors. A non-nonsensical example follows using R syntax on a data frame, returning a vector.

Using data frame syntax on a data frame, data table or spectral object, returning a vector:

```
# not run
sun.spct$s.e.irrad^2 / sun.spct$w.length
```

```
# not run
with(sun.spct, s.e.irrad^2 / w.length)
```

7.7.2 Task: Using operators on underlying vectors

If data for two spectra are available for the same wavelength values, then we can simply use the built in R math operators on the component vectors. These operators are vectorised, which means that an addition between two vectors adds the elements at the same index position in the two vectors with data, in this case for two different spectra.

However, we can achieve the same result, with simpler syntax, using spectral objects and the corresponding operators.

```
sun.spct + sun.spct
```

```
## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 517 more rows
```

```
e2q(sun.spct + sun.spct)
```

```
## Object: source_spct [522 x 3]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Time unit 1s
##
## # A tibble: 522 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## 5 283.6923         0         0
## # ... with 517 more rows
```

In both cases only spectral energy irradiance is calculated during the summing operation, while in the second example, it is simple to convert the returned spectral energy irradiance values into spectral photon irradiance. The class of the returned spectrum depends on the classes of the operands. In this case returned objects are `source_spct`.

The function `oper_spectra` takes the operator to use as an argument, and this abstraction both simplifies the package code, and also makes it easy for users to add other operators if needed:

```
# not run
out.data <- oper_spectra(spc1$w.length, spc2$w.length,
                         spc1$s.e.irrad, spc2$s.e.irrad,
                         bin.oper=`^`)
```

and yields one spectrum to a power of a second one. Such additional functions are not predefined, as I cannot think of any use for them. `oper_spectra` is used internally to define the functions for the four basic maths operators, and the corresponding operators.

7.7.3 Task: conversion from energy to photon base

The energy of a quantum of radiation in a vacuum, q, depends on the wavelength, λ, or frequency[2], ν,

$$q = h \cdot \nu = h \cdot \frac{c}{\lambda} \tag{7.1}$$

with the Planck constant $h = 6.626 \times 10^{-34}$ J s and speed of light in vacuum $c = 2.998 \times 10^{8}$ m s^{-1}. When dealing with numbers of photons, the equation (7.1) can be extended by using Avogadro's number $N_A = 6.022 \times 10^{23}$ mol^{-1}. Thus, the energy of one mole of photons, q', is

$$q' = h' \cdot \nu = h' \cdot \frac{c}{\lambda} \tag{7.2}$$

with $h' = h \cdot N_A = 3.990 \times 10^{-10}$ J s mol^{-1}.

`numeric` vectors

Function `as_quantum` converts W m^{-2} into *number of photons* per square meter per second, and `as_quantum_mol` does the same conversion but returns mol m^{-2} s^{-1}. Function `as_quantum` is based on the equation 7.1 while `as_quantum_mol` uses equation 7.2. To obtain µmol m^{-2} s^{-1} we multiply by 10^6:

```
as_quantum_mol(550, 200) * 1e6

## [1] 919.5147
```

The calculation above is for monochromatic light (200 W m^{-2} at 550 nm).

The functions are vectorised, so they can be applied to whole spectra (when data are available as vectors), to convert W m^{-2} nm^{-1} to mol m^{-2} s^{-1} nm^{-1}:

```
head(sun.spct$s.e.irrad, 10)

##  [1] 0 0 0 0 0 0 0 0 0 0
```

[2] 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 7.1.

```
s.q.irrad <- with(sun.spct,
                  as_quantum_mol(w.length, s.e.irrad))
head(s.q.irrad, 10)

##  [1] 0 0 0 0 0 0 0 0 0 0
```


`source_spct` objects

Once again, easiest is to use spectral objects. The default is to add `s.q.irrad` to the source spectrum, unless it is already present in the object in which case values are not recalculated. It can also be used as a roundabout way of removing a `s.e.irrad` column, which could be useful in some cases.

```
e2q(sun.spct, byref = FALSE)

## Object: source_spct [522 x 3]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## 5 283.6923         0         0
## # ... with 517 more rows
```

`e2q` has a parameter `action`, with default `"add"`. Another valid argument value is `"replace"`.

```
sun.spct

## Object: source_spct [522 x 3]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## 5 283.6923         0         0
## # ... with 517 more rows

e2q(sun.spct, "replace", byref = FALSE)

## Object: source_spct [522 x 2]
```

```
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.q.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 517 more rows
```

`response_spct` objects

In the case of response spectra expressed per energy unit, as the energy unit is a divisor, the conversion is done with the inverse of the factor in equation 7.1. Although the method name is `e2q` as for `source_spct` objects, the appropriate conversion is applied.

7.7.4 Task: conversion from photon to energy base

`as_energy` is the inverse function of `as_quantum_mol`:

`numeric` vectors

In **Aphalo2012** it is written: "Example 1: red light at 600 nm has about 200 $kJ\,mol^{-1}$, therefore, 1 μmol photons has 0.2 J. Example 2: UV-B radiation at 300 nm has about 400 $kJ\,mol^{-1}$, therefore, 1 μmol photons has 0.4 J. Equations 7.1 and 7.2 are valid for all kinds of electromagnetic waves." Let's re-calculate the exact values—as the output from `as_energy` is expressed in $J\,mol^{-1}$ we multiply the result by 10^{-3} to obtain $kJ\,mol^{-1}$:

```
as_energy(600, 1) * 1e-3
```

```
## [1] 199.3805
```

```
as_energy(300, 1) * 1e-3
```

```
## [1] 398.7611
```

Because of vectorization we can also operate on a whole spectrum:

```
s.e.irrad <- with(sun.data, as_energy(w.length, s.q.irrad))
```

`source_spct` objects

Function `q2e` is the reverse of `e2q`, converting spectral energy irradiance in $\mathrm{W\,m^{-2}\,nm^{-1}}$ to spectral photon irradiance in $\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$. It can also be used as a roundabout way of removing a `s.e.irrad` column, which could be useful in some cases.

```
q2e(sun.spct, "replace", byref = FALSE)

## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 517 more rows
```

As we have seen above by default `q2e` and `e2q` return a modified copy of the spectrum as a new object. This is safe, but inefficient in use of memory and computing resources. We first copy the data to a new object, and delete the `s.e.irrad` variable, so that we can test the use of the functions by reference. When parameter `byref` is given `TRUE` as argument the original spectrum is modified.

```
my_sun.spct <- sun.spct
q2e(my_sun.spct, byref = TRUE)

## Object: source_spct [522 x 3]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 522 x 3
##   w.length s.e.irrad s.q.irrad
##      <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## 5 283.6923         0         0
## # ... with 517 more rows
```

`response_spct` objects

In the case of response spectra expressed per energy unit, as the energy unit is a divisor, the conversion is done with the inverse of the factor in equation 7.1. Although

Table 7.2: Options affecting calculations by functions and operators in the 'photobiology' package and their possible values. Options controlling the printing of the returned values are also listed.

Option	default	function
Base R		
digits	7	$d - 3$ used by `summary`
Package 'tibble'		
tibble.print_max	$n_{max} = 20$	nrow(*spct*) $> n_{max}$ print n_{min} lines
tibble.print_min	$n_{min} = 10$	nrow(*spct*) $> n_{max}$ print n_{min} lines
R4photobioloy suite		
photobiology.radiation.unit	`"energy"`	output ($W\,m^{-2}\,nm^{-1}$)
	`"photon"`	output ($mol\,m^{-2}\,s^{-1}\,nm^{-1}$)
photobiology.filter.qty	`"transmittance"`	output (/1)
	`"absorptance"`	output (/1)
	`"absorbance"`	output (a.u. $\log_1 0$ base)
photobiology.use.hinges	`NULL`	guess automatically
	`TRUE`	do not insert hinges
	`FALSE`	do insert hinges
photobiology.auto.hinges.limit	0.5	wavelength step (nm)
photobiology.waveband.trim	`TRUE`	trim or exclude
photobiology.use.cached.mult	`FALSE`	cache intermediate results or not
photobiology.verbose	`FALSE`	give verbose output or not

the method name is `q2e` as for `source_spct` objects, the appropriate conversion is applied.

Task: Using options to change default behaviour of maths operators and functions

Table 7.2 lists all the recognized options, and their default values. Within the suite all functions have a default value which is used when the options are undefined. Options are set using base R's function `options`, and queried with functions `options` and `getOption`. Using options can result in more compact and terse code, but the user should clearly document the use of non-default values for options to avoid surprising the reader of the code.

The behaviour of the operators defined in this package depends on the value of two global options. If we would like the operators to operate on spectral photon irradiance and return spectral photon irradiance instead of spectral energy irradiance, this behaviour can be set, and will remain active until unset or reset.

```
options(photobiology.radiation.unit = "photon")
sun.spct * UVB()

## Object: source_spct [37 x 2]
## Wavelength range 280 to 315 nm, step 0.9230769 to 1 nm
## Time unit 1s
```

```
##
## # A tibble: 37 x 2
##   w.length s.q.irrad
##       <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 32 more rows

options(photobiology.radiation.unit = "energy")
sun.spct * UVB()

## Object: source_spct [37 x 2]
## Wavelength range 280 to 315 nm, step 0.9230769 to 1 nm
## Time unit 1s
##
## # A tibble: 37 x 2
##   w.length s.e.irrad
##       <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 32 more rows
```

For filters, an option controls whether transmittance, the default, or absorbance is use in the operations, and the controls the returned quantity. It is important to remember that absorbance, A, is always expressed on a logarithmic scale, while transmittance, T, is always expressed on a linear scale. So to simulate the effect of stacking two layers of polyester film, we need to sum, or in this case as there are two layers of the same material, multiply by two the spectral absorbance values, while we need to multiply the spectral transmittances of stacked filters, or use a power when the layers are identical.

```
options(photobiology.filter.qty = "absorbance")
polyester.spct * 2

## Object: filter_spct [611 x 2]
## Wavelength range 190 to 800 nm, step 1 nm
##
## # A tibble: 611 x 2
##   w.length        A
##       <int>    <dbl>
## 1      190 3.917215
## 2      191 4.000000
## 3      192 3.917215
## 4      193 3.647817
## 5      194 3.591760
## # ... with 606 more rows

options(photobiology.filter.qty = "transmittance")
polyester.spct ^ 2

## Object: filter_spct [611 x 2]
## Wavelength range 190 to 800 nm, step 1 nm
```

```
##
## # A tibble: 611 x 2
##   w.length      Tfr
##      <int>    <dbl>
## 1      190 0.000121
## 2      191 0.000100
## 3      192 0.000121
## 4      193 0.000225
## 5      194 0.000256
## # ... with 606 more rows
```

Either option can be unset, by means of the `NULL` value[3].

```
options(photobiology.radiation.unit = NULL)
options(photobiology.filter.qty = NULL)
```

The proper use of trimming of wavebands is important, and option `photobiology.waveband.trim` makes changing the behaviour of the `trim_spct` function and other functions accepting wavebands easier. The need to carefully assess the validity of trimming and how it can affect the interpretation of results is further discussed in Chapter 10 and Chapter 11.

Other options affect the optimization of performance vs. precision of calculations and can be useful especially when processing huge numbers of spectra. Some options defined in base R and package 'dplyr' affect printing of output (Table 7.2).

7.8 Wavebands

7.8.1 How are wavebands stored?

Wavebands are derived from R lists. All valid R operations for lists can be also used with `waveband` objects. However, there are `waveband`-specific specializations of generic R methods.

7.8.2 Operators and functions

Multiplying any spectrum by an un-weighted waveband, is equivalent to trimming with `fill` set to `NA` (see section 6.6.3.

```
is_effective(UVA())

## [1] FALSE

sun.spct * UVA()

## Object: source_spct [86 x 2]
## Wavelength range 315 to 400 nm, step 1 nm
## Time unit 1s
##
## # A tibble: 86 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
```

[3] If you are planning to continue working through the examples in later sections, do reset the options as shown in this chunk, as otherwise, the results of later calculations will differ from those shown.

```
## 1      315 0.1127901
## 2      316 0.1020587
## 3      317 0.1487690
## 4      318 0.1413919
## 5      319 0.1569692
## # ... with 81 more rows
```

Multiplying a `source_spct` object by a weighted waveband convolutes the spectrum with weights, yielding effective spectral irradiance.

```
is_effective(CIE())

## [1] TRUE

sun.spct * CIE()

## Object: source_spct [122 x 2]
## Wavelength range 280 to 400 nm, step 0.9230769 to 1 nm
## Time unit 1s
## Data weighted using 'CIE98.298' BSWF
##
## # A tibble: 122 x 2
##   w.length s.e.irrad
##       <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## 5 283.6923         0
## # ... with 117 more rows
```

```
try(detach(package:photobiologyFilters))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

8

Spectra: simple summaries and features

8.1 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)
library(photobiologyWavebands)
library(ggplot2)
library(ggspectra)
library(photobiologyLamps)
library(photobiologyFilters)
library(photobiologyReflectors)
```

8.2 Task: Printing spectra

Spectral objects are printed with a special `print` method that is an extension to the print method for `tibble` objects, consequently, it is possible to use options from package 'tibble' to control printing. The first option set below, `tibble.print_max`, sets the number of rows above which only 'head' rows are printed and `tibble.print_min` sets the number of rows printed when the head is printed. Another option, `tibble.width` sets width of the output printed for `tibble` objects with many columns.

```
options(tibble.print_max = 4, tibble.print_min = 4)
```

The number of rows printed can be also controlled through an explicit argument to the second parameter of `print`, `head`, and `tail`. Setting an option by means of `options` changes the default behaviour of `print`, but explicit arguments can still be used for changing this behaviour in an individual statement.

8.3 Task: Summaries related to object properties

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)

## Summary of object: source_spct [522 x 3]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit: 1s
##
##     w.length       s.e.irrad
##  Min.   :280.0   Min.   :0.0000
##  1st Qu.:409.2   1st Qu.:0.4115
##  Median :539.5   Median :0.5799
##  Mean   :539.5   Mean   :0.5160
##  3rd Qu.:669.8   3rd Qu.:0.6664
##  Max.   :800.0   Max.   :0.8205
##    s.q.irrad
##  Min.   :0.000e+00
##  1st Qu.:1.980e-06
##  Median :2.929e-06
##  Mean   :2.407e-06
##  3rd Qu.:3.154e-06
##  Max.   :3.375e-06
```

8.4 Task: Integrating spectral data

Package 'photobiology' provides specific functions for frequently used quantities, but in addition 'general purpose' function is available to add flexibility for special cases. Function `integrate_spct` takes into account each individual wavelength step, so it returns valid results even for spectra measured at arbitrary and varying wavelength steps. This function operates on all `numeric` variables contained in a spectral object except for `w.length`. The returned value is expressed as a total per spectrum.

```
integrate_spct(sun.spct)

##      e.irrad      q.irrad
## 2.691249e+02 1.255336e-03
```

8.5 Task: Averaging spectral data

Package 'photobiology' provides specific functions for frequently used quantities, but in addition 'general purpose' function is available to add flexibility for special cases. Function `average_spct` takes into account each individual wavelength step, so it returns valid results even for spectra measured at arbitrary and varying wavelength steps. This function operate on all `numeric` variables contained in a spectral object except for `w.length`. The returned value is expressed per nanometre.

```
average_spct(sun.spct)

##      e.irrad      q.irrad
## 5.175479e-01 2.414107e-06
```

8.6 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] 280 800

midpoint(sun.spct)

## [1] 540

max(sun.spct)

## [1] 800

min(sun.spct)

## [1] 280
```

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] 520

stepsize(sun.spct)

## [1] 0.9230769 1.0000000
```

8.7 Task: Finding the class of an object

R method `class` can be used with any R object, including spectra.

```
class(sun.spct)

## [1] "source_spct"  "generic_spct" "tbl_df"
## [4] "tbl"          "data.frame"

class(polyester.spct)

## [1] "filter_spct"  "generic_spct" "tbl_df"
## [4] "tbl"          "data.frame"
```

The method `class_spct` is a convenience wrapped on `class` which returns only class attributes corresponding to spectral classes defined in package 'photobiology'.

```
class_spct(sun.spct)

## [1] "source_spct"  "generic_spct"

class_spct(polyester.spct)

## [1] "filter_spct"  "generic_spct"
```

The method `is.any_spct` is a synonym of `is.generic_spct` as `generic_spct` is the base class from which all spectral classes are derived.

```
is.any_spct(sun.spct)

## [1] TRUE

is.any_spct(polyester.spct)

## [1] TRUE
```

Equivalent methods exist for all the classes defined in package 'photobiology'. We show two examples below, with a radiation source and a filter.

```
is.source_spct(sun.spct)

## [1] TRUE

is.source_spct(polyester.spct)

## [1] FALSE
```

```
is.filter_spct(sun.spct)

## [1] FALSE

is.filter_spct(polyester.spct)

## [1] TRUE
```

8.8 Task: Querying other attributes

Both `response_spct` and `source_spct` objects have an attribute `time.unit` that can be queried.

```
getTimeUnit(sun.spct)

## [1] "second"
```

```
is_effective(sun.spct * CIE())

## [1] TRUE

is_effective(sun.spct * UV())

## [1] FALSE
```

```
getBSWFUsed(sun.spct * CIE())

## [1] "CIE98.298"
```

Normalization and scaling can be applied to different types of spectral objects.

```
sun.norm.spct <- normalize(sun.spct, norm = 600)
is_normalized(sun.norm.spct)

## [1] TRUE

getNormalized(sun.norm.spct)

## [1] 600
```

```
sun.scaled.spct <- fscale(sun.spct, f = "mean")
is_scaled(sun.scaled.spct)

## [1] TRUE
```

We now consider `filter_spct` objects (see Chapter 12 for an explanation of the meaning of these attributes and how they affect calculations).

```
getTfrType(polyester.spct)

## [1] "total"
```

and `reflector_spct` objects.

```
getRfrType(gold.spct)

## [1] "total"
```

8.9 Task: Query how spectral data contained is expressed

We first consider the case of `source.spct` objects. If an object contains the same data expressed differently, it is possible, as in the example for both statement to return true.

```
head(sun.spct)

## Object: source_spct [6 x 3]
## Wavelength range 280 to 284.61538 nm, step 0.9230769 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 6 x 3
##   w.length s.e.irrad s.q.irrad
## *    <dbl>     <dbl>     <dbl>
## 1 280.0000         0         0
## 2 280.9231         0         0
## 3 281.8462         0         0
## 4 282.7692         0         0
## # ... with 2 more rows
```

```
is_energy_based(sun.spct)

## [1] TRUE

is_photon_based(sun.spct)

## [1] TRUE
```

If we delete the energy based spectral data, the result of the test changes.

```
my.spct <- sun.spct
my.spct$s.e.irrad <- NULL
head(my.spct)

## Object: source_spct [6 x 2]
## Wavelength range 280 to 284.61538 nm, step 0.9230769 nm
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.20942 N, 24.96424 E
## Time unit 1s
##
## # A tibble: 6 x 2
##   w.length s.q.irrad
## *    <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.8462         0
## 4 282.7692         0
## # ... with 2 more rows

is_energy_based(my.spct)

## [1] FALSE

is_photon_based(my.spct)

## [1] TRUE
```

We now consider `filter_spct` objects.

```
is_transmittance_based(polyester.spct)

## [1] TRUE

is_absorbance_based(polyester.spct)

## [1] FALSE
```

8.10 Task: Querying about 'origin' of data

All spectral objects (`generic_spct` and derived types) can be queried whether they are the result of the normalization or re-scaling of another spectrum. In the case of normalization, the normalization wavelength in nanometres is returned, otherwise a logical value.

```
is_normalized(sun.spct)

## [1] FALSE

is_scaled(sun.spct)

## [1] FALSE
```

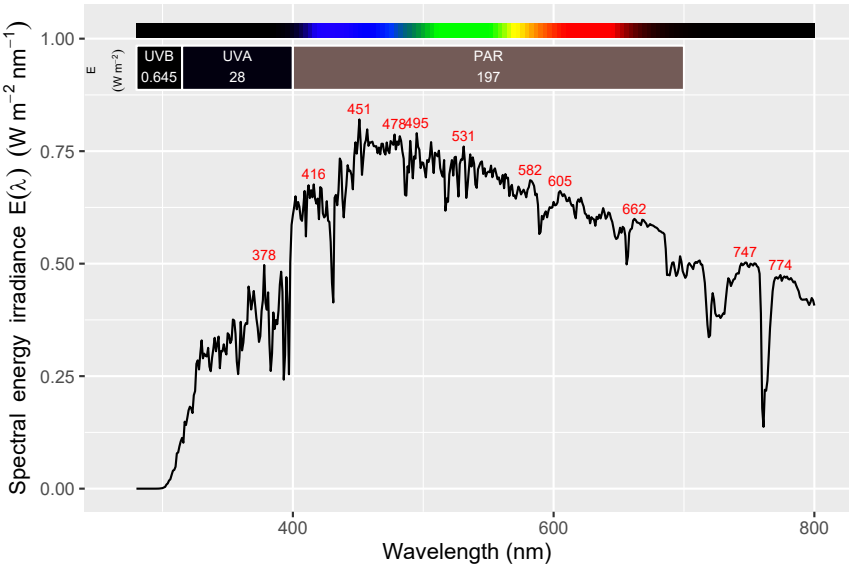

`source_spct` objects can be queried to learn if they are the result of a calculation involving a weighting function.

```
is_effective(sun.spct)

## [1] FALSE
```

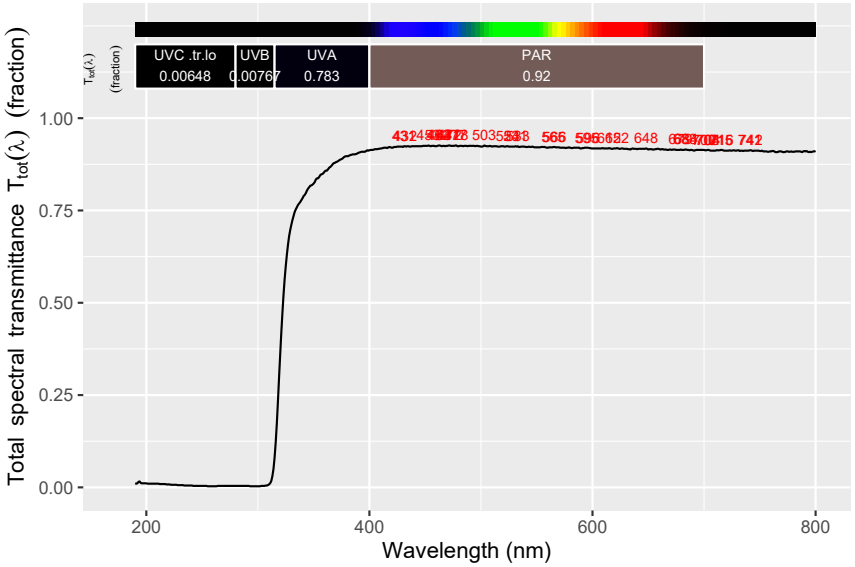
8.11 Task: Plotting a spectrum

Method `plot` is defined for `waveband` objects, and can be used to visually check their properties. Plotting is discussed in detail in chapter ??.

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




```
plot(polyester.spct)
```



8.12 Task: Other R's methods

Methods `names` and `comment` should work as usual. In the case of the comment attribute, most operations on spectral objects preserve comments, sometimes with additions, or by merging of comments from operands. Comments are optional, so for some objects `comment` may return a `NULL`. As some comments contain new line characters, to get them printed nicely we need to use `cat`.

```
names(sun.spct)

## [1] "w.length"  "s.e.irrad" "s.q.irrad"

cat(comment(sun.spct))

## Simulated solar spectrum based on real weather conditions.
## Data author: Dr. Anders Lindfors
## Finnish Meteorological Institute.
## See help file for references.
```

8.13 Task: Find peaks and valleys

Methods `peaks` and `valleys` can be used on most spectral objects to find local maxima and local minima in spectral data. They return an object of the same class containing only the observations corresponding to these local extremes.

```
peaks(philips.tl12.spct)

## Object: source_spct [30 x 2]
## Wavelength range 313 to 730 nm, step 4 to 52 nm
```

```
## Time unit 1s
##
## # A tibble: 30 x 2
##   w.length s.e.irrad
## *    <int>     <dbl>
## 1      313   0.29181
## 2      365   0.06587
## 3      391   0.00202
## 4      404   0.15675
## # ... with 26 more rows
```

```
peaks(philips.tl12.spct, unit.out = "photon")
```

```
## Object: source_spct [31 x 2]
## Wavelength range 313 to 730 nm, step 4 to 52 nm
## Time unit 1s
##
## # A tibble: 31 x 2
##   w.length    s.q.irrad
## *    <int>        <dbl>
## 1      313 7.635026e-07
## 2      365 2.009771e-07
## 3      391 6.602283e-09
## 4      404 5.293646e-07
## # ... with 27 more rows
```

```
peaks(philips.tl12.spct, span = 50)
```

```
## span increased to next odd value:  51
## Object: source_spct [10 x 2]
## Wavelength range 313 to 730 nm, step 31 to 79 nm
## Time unit 1s
##
## # A tibble: 10 x 2
##   w.length s.e.irrad
## *    <int>     <dbl>
## 1      313   0.29181
## 2      365   0.06587
## 3      404   0.15675
## 4      435   0.38773
## # ... with 6 more rows
```

```
valleys(schott.mspct$KG5)
```

```
## Object: filter_spct [6 x 2]
## Wavelength range 424 to 3000 nm, step 34 to 900 nm
##
## # A tibble: 6 x 2
##   w.length          Tfr
## *    <dbl>        <dbl>
## 1      424 8.478600e-01
## 2      458 8.615100e-01
## 3      529 8.742400e-01
## 4     1250 6.823387e-06
## # ... with 2 more rows
```

```
peaks(schott.mspct$KG5, filter.qty = "absorbance")
```

```
## Object: filter_spct [6 x 2]
```

```
## Wavelength range 424 to 3000 nm, step 34 to 900 nm
##
## # A tibble: 6 x 2
##   w.length          A
## *    <dbl>      <dbl>
## 1      424 0.07167585
## 2      458 0.06473968
## 3      529 0.05836933
## 4     1250 5.16600000
## # ... with 2 more rows
```

8.13.1 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.

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

```
## [1] FALSE FALSE FALSE FALSE FALSE FALSE
```

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

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

```
## [1] 37 39 43 49 52 54
```

8.13.2 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, span = 51))[["x"]]
```

```
## [1] 451 495 747
```

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

8.14 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.

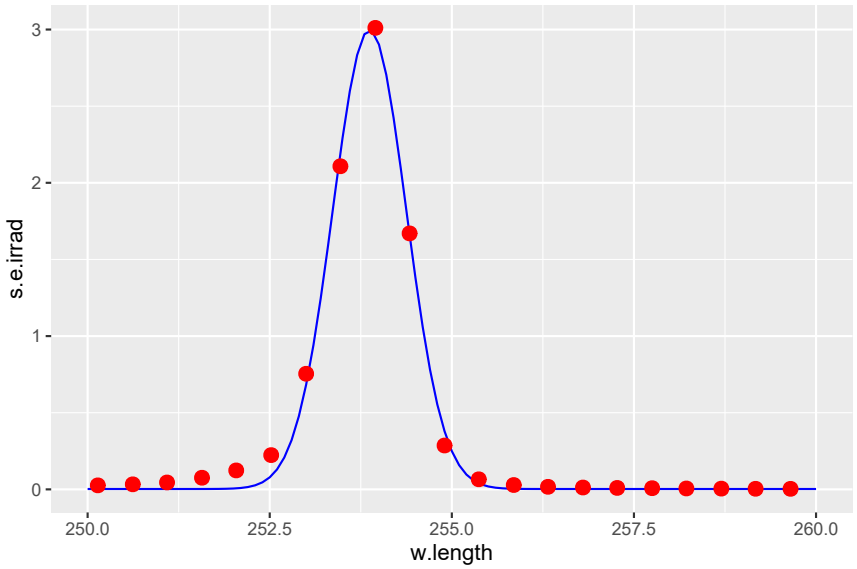
```
stepsize(germicidal.spct)

## [1] 0.43 0.48

peaks <-
   with(germicidal.spct,
        get_peaks(w.length, s.e.irrad, span = 5))
fit <- nls(s.e.irrad ~ d + a1*exp(-0.5*((w.length-c1)/b1)^2),
           start=list(a1=3.1, b1=1, c1=peaks[1, 1], d=0),
           data=germicidal.spct)
fit

## Nonlinear regression model
##   model: s.e.irrad ~ d + a1 * exp(-0.5 * ((w.length - c1)/b1)^2)
##    data: germicidal.spct
##        a1        b1        c1         d
## 2.996e+00 5.056e-01 2.539e+02 2.386e-03
##  residual sum-of-squares: 0.1309
##
## Number of iterations to convergence: 6
## Achieved convergence tolerance: 6.219e-06

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

## [1] 253.8703

peaks[1, 1]

## [1] 253.95
```

In this case the change was rather small, and shows a small wavelength calibration error for the spectrometer that can be calculated as:

```
signif(fit$m$getPars()[["c1"]], 6) - 253.652

## [1] 0.218
```

```
predicted <-
  predict(fit,
          data.frame(w.length = seq(250, 260, length.out = 101)))
fitted_peak.spct <-
  source_spct(w.length  = seq(250, 260, length.out = 101),
              s.e.irrad = predicted)
```

```
ggplot(data = fitted_peak.spct, aes(w.length, s.e.irrad)) +
  geom_line(data = fitted_peak.spct, colour = "blue") +
  geom_point(data = germicidal.spct, colour = "red", size = 3) +
  xlim(250, 260)

## Warning: Removed 1404 rows containing missing values
## (geom_point).
```




```
try(detach(package:photobiologyReflectors))
try(detach(package:photobiologyFilters))
try(detach(package:photobiologyLamps))
try(detach(package:ggspectra))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

9

Wavebands: simple summaries and features

9.1 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)
library(photobiologyWavebands)
library(ggspectra)
```

9.2 Task: Printing spectra

A `print` method for `waveband` objects is defines in package 'photobiology', which in the example below is called implicitly.

```
VIS()

## VIS.ISO
## low (nm) 380
## high (nm) 760
## weighted none

CIE()

## CIE98.298
## low (nm) 250
## high (nm) 400
## weighted SWF
## normalized at 298 nm
```

To print the internals (the underlying components) of the object, one can use method `unclass`.

```
unclass(VIS())

## $low
## [1] 380
##
## $high
## [1] 760
##
## $weight
## [1] "none"
##
## $SWF.e.fun
```

```
## NULL
##
## $SWF.q.fun
## NULL
##
## $SWF.norm
## NULL
##
## $norm
## NULL
##
## $hinges
## [1] 380 380 760 760
##
## $name
## [1] "VIS.ISO"
##
## $label
## [1] "VIS"
```

```
unclass(CIE())
```

```
## $low
## [1] 250
##
## $high
## [1] 400
##
## $weight
## [1] "SWF"
##
## $SWF.e.fun
## function (w.length)
## {
##     CIE.energy <- numeric(length(w.length))
##     CIE.energy[w.length <= 298] <- 1
##     CIE.energy[(w.length > 298) & (w.length <= 328)] <- 10^(0.094 *
##         (298 - w.length[(w.length > 298) & (w.length <= 328)]))
##     CIE.energy[(w.length > 328) & (w.length <= 400)] <- 10^(0.015 *
##         (139 - w.length[(w.length > 328) & (w.length <= 400)]))
##     CIE.energy[w.length > 400] <- 0
##     return(CIE.energy)
## }
## <bytecode: 0x000000001aba6818>
## <environment: namespace:photobiologyWavebands>
##
## $SWF.q.fun
## function (w.length)
## {
##     SWF.e.fun(w.length) * SWF.norm/w.length
## }
## <bytecode: 0x0000000014810c48>
## <environment: 0x00000000172df708>
##
## $SWF.norm
## [1] 298
##
## $norm
## [1] 298
##
## $hinges
```

```
## [1] 250 250 298 328 400 400
##
## $name
## [1] "CIE98.298"
##
## $label
## [1] "CIE98"
```

9.3 Task: Summaries related to object properties

In the case of the `summary` method and their corresponding print method, specializations for all classes of spectral objects are provided—i.e. all classes with names ending in `_spct`.

```
my.wb <- waveband(c(400,500))
summary(my.wb)

##           Length Class  Mode
## low       1      -none- numeric
## high      1      -none- numeric
## weight    1      -none- character
## SWF.e.fun 0      -none- NULL
## SWF.q.fun 0      -none- NULL
## SWF.norm  0      -none- NULL
## norm      0      -none- NULL
## hinges    4      -none- numeric
## name      1      -none- character
## label     1      -none- character
```

```
vis.wb <- VIS()
summary(vis.wb)

##           Length Class  Mode
## low       1      -none- numeric
## high      1      -none- numeric
## weight    1      -none- character
## SWF.e.fun 0      -none- NULL
## SWF.q.fun 0      -none- NULL
## SWF.norm  0      -none- NULL
## norm      0      -none- NULL
## hinges    4      -none- numeric
## name      1      -none- character
## label     1      -none- character
```

```
cie.wb <- CIE()
summary(cie.wb)

##           Length Class  Mode
## low       1      -none- numeric
## high      1      -none- numeric
## weight    1      -none- character
## SWF.e.fun 1      -none- function
## SWF.q.fun 1      -none- function
## SWF.norm  1      -none- numeric
```

```
## norm      1      -none- numeric
## hinges    6      -none- numeric
## name      1      -none- character
## label     1      -none- character
```

9.4 Task: Summaries related to wavelength

Functions `max`, `min`, `range`, `midpoint` when used with an object of class `waveband` return the result of applying these functions to the wavelength component boundaries of these objects, returning always values expressed in nanometres as long as the objects have been correctly created.

```
range(vis.wb)

## [1] 380 760

midpoint(vis.wb)

## [1] 570

max(vis.wb)

## [1] 760

min(vis.wb)

## [1] 380
```

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(vis.wb)

## [1] 380
```

9.5 Task: Querying other properties

It is possible to query whether a `waveband` object includes a weighting function using function `is_effective`. Weighting functions are used for the calculation *effective irradiances* and *effective exposures*.

```
is_effective(vis.wb)

## [1] FALSE

is_effective(cie.wb)

## [1] TRUE
```

9.6 Task: R's methods

The "labels" can be retrieved with R's method `labels`. Waveband objects have two slots for names, normally used when wavebands are plotted or printed.

```
labels(my.wb)

## $label
## [1] "range.400.500"
##
## $name
## [1] "range.400.500"

labels(vis.wb)

## $label
## [1] "VIS"
##
## $name
## [1] "VIS.ISO"

labels(cie.wb)

## $label
## [1] "CIE98"
##
## $name
## [1] "CIE98.298"
```

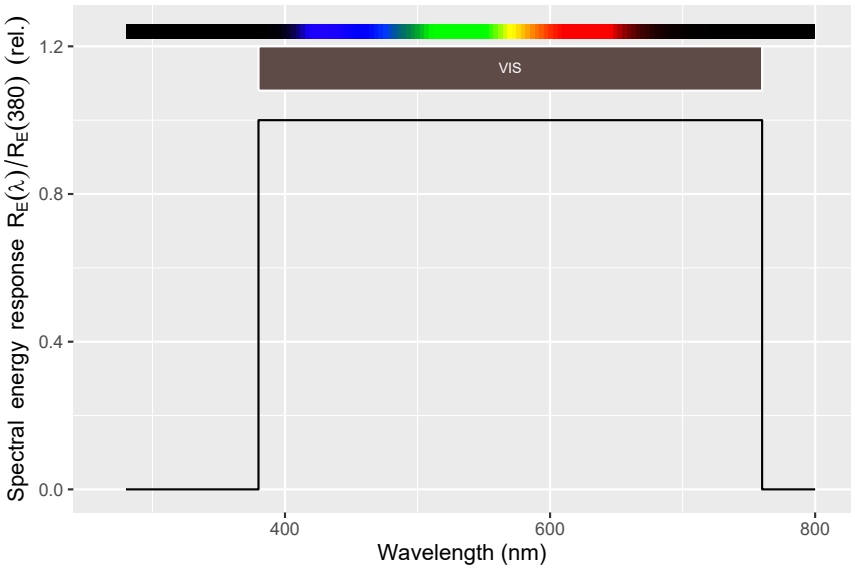
As with any R object, method `names` returns a vector of names of the object's components.

```
names(vis.wb)

##  [1] "low"       "high"      "weight"
##  [4] "SWF.e.fun" "SWF.q.fun" "SWF.norm"
##  [7] "norm"      "hinges"    "name"
## [10] "label"

names(cie.wb)

##  [1] "low"       "high"      "weight"
##  [4] "SWF.e.fun" "SWF.q.fun" "SWF.norm"
##  [7] "norm"      "hinges"    "name"
## [10] "label"
```

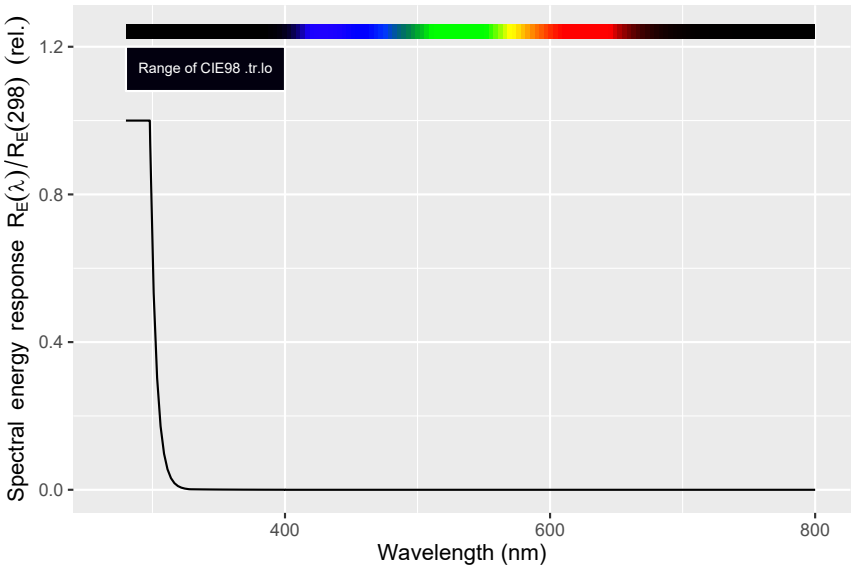
9.7 Task: Plotting a waveband

Method `plot` is defined for `waveband` objects, and can be used to visually check their properties. Plotting is discussed in detail in chapter ??.

```
plot(vis.wb)
```




```
plot(cie.wb)
```




```
try(detach(package:ggspectra))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

10

Unweighted irradiance

10.1 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)
library(photobiologyWavebands)
library(photobiologyLamps)
library(photobiologyLEDs)
library(lubridate)
```

10.2 Introduction

Functions `e_irrad` and `q_irrad` return energy irradiance and photon (or quantum) irradiance, and both take as argument a `source_spct` object containing either spectral (energy) irradiance or spectral photon irradiance data. An additional parameter accepting a `waveband` object, or a list of `waveband` objects, can be used to set the range(s) of wavelengths and spectral weighting function(s) to use for integration(s). Two additional functions, `energy_irradiance` and `photon_irradiance`, are defined for equivalent calculations on spectral irradiance data stored as numeric vectors.

We start by describing how to use and define `waveband` objects, for which we need to use function `e_irrad` in some examples before a detailed explanation of its use (see section 10.6) on page 106 for details).

10.3 Task: use simple predefined wavebands

Please, consult the packages' documentation for a list of predefined functions for creating wavebands also called `waveband` *constructors*. 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 100

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
## weighted none
```

As seen above, there is a specialized `print` method for `wavebands`. `waveband` methods returning wavelength values in nm are `min`, `max`, `range`, `midpoint`, and `spread`. Method `labels` returns the name and label stored in the waveband, and method `color` returns a color definition calculated from the range of wavelengths.

```
red <- Red()
red

## Red.ISO
## low (nm) 610
## high (nm) 760
## weighted none

min(red)

## [1] 610

max(red)

## [1] 760

range(red)

## [1] 610 760

midpoint(red)

## [1] 685

spread(red)

## [1] 150

labels(red)

## $label
## [1] "Red"
##
## $name
## [1] "Red.ISO"

color(red)

##   Red.CMF
## "#900000"
```

The argument `standard` can be used to choose a given alternative definition[1]:

```
UVB()
```

[1] When available, the definition in the ISO standard is the default.

```
## UVB.ISO
## low (nm) 280
## high (nm) 315
## weighted none

UVB("ISO")

## UVB.ISO
## low (nm) 280
## high (nm) 315
## weighted none

UVB("CIE")

## UVB.CIE
## low (nm) 280
## high (nm) 315
## weighted none

UVB("medical")

## UVB.medical
## low (nm) 290
## high (nm) 320
## weighted none

UVB("none")

## UVB.none
## low (nm) 280
## high (nm) 320
## weighted none
```

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

```
e_irrad(sun.spct, UVB("ISO"))

##   UVB.ISO
## 0.6445105
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"

e_irrad(sun.spct, UVB("none"))

##  UVB.none
##  1.337179
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"

e_irrad(sun.spct, UVB("ISO")) / e_irrad(sun.spct, UVB("none"))

##   UVB.ISO
## 0.4819927
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

10.4 Task: define simple wavebands

Here we briefly introduce `waveband` and `new_waveband`, and only in chapter **??** we describe their use in full detail, including the use of spectral weighting functions (SWFs). The examples in the present section only describe `waveband`s that define a wavelength range.

A `waveband` can be created based on any R object for which function `range` is defined, and returns numbers interpretable as wavelengths expressed in nanometres:

```
waveband(c(400,700))

## range.400.700
## low (nm) 400
## high (nm) 700
## weighted none

waveband(400:700)

## range.400.700
## low (nm) 400
## high (nm) 700
## weighted none

waveband(sun.spct)

## Total
## low (nm) 280
## high (nm) 800
## weighted none

wb_total <- waveband(sun.spct, wb.name="total")
```

```
e_irrad(sun.spct, wb_total)

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

A `waveband` can also be created based on extreme wavelengths expressed in nm.

```
wb1 <- new_waveband(500,600)
wb1

## range.500.600
## low (nm) 500
## high (nm) 600
## weighted none

e_irrad(sun.spct, wb1)

##  range.500.600
##        68.4895
## attr(,"time.unit")
```

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

wb2 <- new_waveband(500,600, wb.name="my.colour")
wb2

## my.colour
## low (nm) 500
## high (nm) 600
## weighted none

e_irrad(sun.spct, wb2)

##  my.colour
##    68.4895
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```


10.5 Task: define lists of simple wavebands

Lists of wavebands can be created by grouping `waveband` objects using the R-defined constructor `list`,

```
UV.list <- list(UVC(), UVB(), UVA())
UV.list

## [[1]]
## UVC.ISO
## low (nm) 100
## high (nm) 280
## weighted none
##
## [[2]]
## UVB.ISO
## low (nm) 280
## high (nm) 315
## weighted none
##
## [[3]]
## UVA.ISO
## low (nm) 315
## high (nm) 400
## weighted none
```

in which case wavebands can be non-contiguous and/or overlapping.

In addition function `split_bands` can be used to create a list of contiguous wavebands by supplying a numeric vector of wavelength boundaries in nanometres,

```
split_bands(c(400,500,600))

## $wb1
## range.400.500
```

```
## low (nm) 400
## high (nm) 500
## weighted none
##
## $wb2
## range.500.600
## low (nm) 500
## high (nm) 600
## weighted none
```

or with longer but more meaningful names,

```
split_bands(c(400,500,600), short.names=FALSE)

## $range.400.500
## range.400.500
## low (nm) 400
## high (nm) 500
## weighted none
##
## $range.500.600
## range.500.600
## low (nm) 500
## high (nm) 600
## weighted none
```

It is also possible to also provide the limits of the region to be covered by the list of wavebands and the number of (equally spaced) wavebands desired:

```
split_bands(c(400,600), length.out=2)

## $wb1
## range.400.500
## low (nm) 400
## high (nm) 500
## weighted none
##
## $wb2
## range.500.600
## low (nm) 500
## high (nm) 600
## weighted none
```

in all cases coderange is used to find the list boundaries, so we can also split the region defined by an existing `waveband` object into smaller wavebands,

```
split_bands(PAR(), length.out=3)

## $wb1
## range.400.500
## low (nm) 400
## high (nm) 500
## weighted none
##
## $wb2
## range.500.600
## low (nm) 500
## high (nm) 600
```

```
## weighted none
##
## $wb3
## range.600.700
## low (nm) 600
## high (nm) 700
## weighted none
```

or split a whole spectrum[2] into equally sized regions,

```
split_bands(sun.spct, length.out=3)

## $wb1
## range.280.453.3
## low (nm) 280
## high (nm) 453
## weighted none
##
## $wb2
## range.453.3.626.7
## low (nm) 453
## high (nm) 627
## weighted none
##
## $wb3
## range.626.7.800
## low (nm) 627
## high (nm) 800
## weighted none
```

It is also possible to supply a list of wavelength ranges[3], and, when present, names are copied from the input list to the output list:

```
split_bands(list(c(400,500), c(600,700)))

## $wb.a
## range.400.500
## low (nm) 400
## high (nm) 500
## weighted none
##
## $wb.b
## range.600.700
## low (nm) 600
## high (nm) 700
## weighted none

split_bands(list(blue=c(400,500), PAR=c(400,700)))

## $blue
## range.400.500
## low (nm) 400
## high (nm) 500
## weighted none
##
```

[2] This is not restricted to `source_spct` objects as all other classes of `___.spct` objects also have `range` methods defined.

[3] When using a list argument, even overlapping and non-contiguous wavelength ranges are valid input

```
## $PAR
## range.400.700
## low (nm) 400
## high (nm) 700
## weighted none
```

Package 'photobiologyWavebands' also predefines some useful constructors of lists of wavebands, currently `VIS_bands`, `UV_bands` and `Plant_bands`.

```
UV_bands()

## [[1]]
## UVC.ISO
## low (nm) 100
## high (nm) 280
## weighted none
##
## [[2]]
## UVB.ISO
## low (nm) 280
## high (nm) 315
## weighted none
##
## [[3]]
## UVA.ISO
## low (nm) 315
## high (nm) 400
## weighted none
```

10.6 Task: (energy) irradiance from spectral irradiance

The task to be completed is to calculate the (energy) irradiance (E) in $\mathrm{W\,m^{-2}}$ from spectral (energy) irradiance ($E(\lambda)$) in $\mathrm{W\,m^{-2}\,nm^{-1}}$ and the corresponding wavelengths (λ) in nm.

$$E_{\lambda_1<\lambda<\lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda)\,\mathrm{d}\lambda \tag{10.1}$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) energy irradiance, for which the most accepted limits are $\lambda_1 = 400\mathrm{nm}$ and $\lambda_1 = 700\mathrm{nm}$. In this example we will use example data for sunlight to calculate $E_{400\,\mathrm{nm}<\lambda<700\,\mathrm{nm}}$. The function used for this task when working with spectral objects is `e_irrad` returning energy irradiance. The "names" of the returned valued is set according to the waveband used, and `sun.spct` is a `source_spct` object.

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

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

or using the `PAR` waveband constructor, defined in package 'photobiologyWavebands' as a convenience function,

```
e_irrad(sun.spct, PAR())

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

or if no waveband is supplied as argument, then irradiance is computed for the whole range of wavelengths in the spectral data, and the 'name' attribute is generated accordingly.

```
e_irrad(sun.spct)

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

If a waveband extends outside of the wavelength range of the spectral data, spectral irradiance for unavailable wavelengths is assumed to be zero:

```
e_irrad(sun.spct, waveband(c(100,400)))

##  range.100.400.tr.lo
##              28.62872
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"

e_irrad(sun.spct, waveband(c(100,250)))

## Warning in is.na(x): is.na() applied to non-(list or vector) of type 'NULL'

## out of range
##            NA
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

Both `e_irrad` and `q_irrad` accept, in addition to a waveband as second argument, a list of wavebands. In this case, the returned value is a numeric vector of the same length as the list.

```
e_irrad(sun.spct, list(UVB(), UVA()))

##    UVB.ISO    UVA.ISO
##  0.6445105 27.9842061
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

Storing emission spectral data in `source_spct` objects is recommended, as it allows better protection against mistakes, and allows automatic detection of input data base of expression and units. However, it may be sometimes more convenient or efficient to keep spectral data in individual numeric vectors, or data frames. In such cases function `energy_irradiance`, which accepts the spectral data as vectors can be used at the cost of less concise code and weaker error tests. In this case, the user must indicate whether spectral data is on energy or photon based units through parameter `unit.in`, which defaults to `"energy"`.

For example when using function `PAR()`, the code above becomes:

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

##      PAR
## 196.6343

with(sun.spct,
     energy_irradiance(w.length, s.e.irrad, PAR(), unit.in="energy"))

##      PAR
## 196.6343
```

where `sun.spct` is a data frame. However, the data can also be stored in separate numeric vectors of equal length.

The `sun.spct` data frame also contains spectral photon irradiance values:

```
names(sun.spct)

## [1] "w.length"  "s.e.irrad" "s.q.irrad"
```

which allows us to use:

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

##      PAR
## 196.6343
```

The other examples above can be re-written with similar syntax.

10.7 Task: photon irradiance from spectral irradiance

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

Combining equations 10.3 and **??** we obtain:

$$Q_{\lambda_1<\lambda<\lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda)\ \frac{h' \cdot c}{\lambda}\ \mathrm{d}\lambda \tag{10.2}$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) photon irradiance (frequently called PPFD or photosynthetic photon flux density), for which the most accepted limits are $\lambda_1 = 400\mathrm{nm}$ and $\lambda_1 = 700\mathrm{nm}$. In this example we

will use example data for sunlight to calculate $E_{400\,\mathrm{nm}<\square<700\,\mathrm{nm}}$. The function used for this task when working with spectral objects is `q_irrad`, returning photon irradiance in $\mathrm{mol\,m^{-2}\,s^{-1}}$. The "names" of the returned valued is set according to the waveband used, and `sun.spct` is a `source_spct` object.

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

##  range.400.700
##   0.0008941352
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

to obtain the photon irradiance expressed in $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$ we multiply the returned value by 1×10^6:

```
q_irrad(sun.spct, waveband(c(400,700))) * 1e6

##  range.400.700
##       894.1352
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

or using the `PAR` waveband constructor, defined in package 'photobiologyWavebands' as a convenience function,

```
q_irrad(sun.spct, PAR()) * 1e6

##      PAR
## 894.1352
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

Examples given in section 10.6 can all be converted by replacing `e_irrad` function calls with `q_irrad` function calls.

Storing emission spectral data in `source_spct` objects is recommended (see section 10.6). However, it may be sometimes more convenient or efficient to keep spectral data in individual numeric vectors, or data frames. In such cases function `photon_irradiance`, which accepts the spectral data as vectors can be used at the cost of less concise code and weaker error tests. In this case, the user must indicate whether spectral data is on energy or photon based units through parameter `unit.in`, which defaults to `"energy"`.

For example when using function `PAR()`, the code above becomes:

```
with(sun.spct,
     photon_irradiance(w.length, s.e.irrad, PAR()), unit.in="energy")  * 1e6

##      PAR
## 894.1352
```

```
with(sun.spct,
     photon_irradiance(w.length, s.e.irrad, PAR()))  * 1e6

##      PAR
## 894.1352
```

where `sun.spct` is a data frame. However, the data can also be stored in separate numeric vectors of equal length.

10.8 Task: irradiance for more than one waveband

As discussed above, it is possible to calculate simultaneously the irradiance for several wavebands with a single function call by supplying a `list` of `wavebands` as argument:

```
q_irrad(sun.spct, list(Red(), Green(), Blue())) * 1e6

##    Red.ISO  Green.ISO   Blue.ISO
##   451.1083   220.1957   149.0288
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

Q.RGB <- q_irrad(sun.spct, list(Red(), Green(), Blue())) * 1e6
signif(Q.RGB, 3)

##    Red.ISO  Green.ISO   Blue.ISO
##        451        220        149
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

Q.RGB[1]

##  Red.ISO
## 451.1083

Q.RGB["Green.ISO"]

## <NA>
##   NA
```

as the value returned is in $\mathrm{mol\,m^{-2}\,s^{-1}}$ we multiply it by 1×10^6 to obtain $\mu\mathrm{mol\,m^{-2}\,s^{-1}}$.

A named list can be used to override the names used for the output:

```
q_irrad(sun.spct, list(R=Red(), G=Green(), B=Blue())) * 1e6

##    Red.ISO  Green.ISO   Blue.ISO
##   451.1083   220.1957   149.0288
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

Even when using a single waveband:

```
q_irrad(sun.spct, list('ultraviolet-B'=UVB())) * 1e6

##  UVB.ISO
## 1.675362
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

The examples above, can be easily rewritten using functions `e_irrad`, `energy_irradiance` or `photon_irradiance`.

For example, the second example above becomes:

```
e_irrad(sun.spct, list(R=Red(), G=Green(), B=Blue()))

##    Red.ISO  Green.ISO   Blue.ISO
##   79.38159   49.26860   37.55207
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

or

```
with(sun.spct,
     energy_irradiance(w.length, s.e.irrad,
                       list(R=Red(), G=Green(), B=Blue())))

##        R        G        B
## 79.38159 49.26860 37.55207
```

10.9 Task: calculate fluence for an irradiation event

The task to be completed is to calculate the (energy) fluence (F) in J from spectral (energy) irradiance ($E(\lambda)$) in $\mathrm{W\,m^{-2}\,nm^{-1}}$ and the corresponding wavelengths (λ) in nm.

$$F_{\lambda_1<\lambda<\lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda) \times t \, \mathrm{d}\lambda \tag{10.3}$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) energy irradiance, for which the most accepted limits are $\lambda_1 = 400\mathrm{nm}$ and $\lambda_1 = 700\mathrm{nm}$. In this example we will use example data for sunlight to calculate $E_{400\,\mathrm{nm}<\lambda<700\,\mathrm{nm}}$. The function used for this task when working with spectral objects is `e_irrad` returning energy irradiance. The "names" of the returned valued is set according to the waveband used, and `sun.spct` is a `source_spct` object. The use of function `fluence` facilitates the calculation as it accepts the length of time of the exposure as a `lubridate::duration`, making it easy to enter the duration using different units, or even calculate the duration as the difference between two times. Of course, the spectral irradiance should be measured at the position where the material being exposed

was located during irradiation. The following example is for a red fluorescent tube as sometimes used in seed germination experiments to study phytochrome-mediated responses.

```
fluence(philips.tld36w.15.spct,
        exposure.time = duration(5, "minutes"))

##    Total
## 301.4848
## attr(,"radiation.unit")
## [1] "energy fluence (J m-2)"
## attr(,"exposure.duration")
## [1] "300s (~5 minutes)"
```

Please see the sections 11.8 for additional details.

10.10 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 red to far-red photon ratio (R:FR photon ratio or ζ). If we follow the wavelength ranges in the definition given by **Morgan1981a** using photon irradiance[4]:

$$\zeta = \frac{Q_{655\text{nm}<\square<665\text{nm}}}{Q_{725\text{nm}<\square<735\text{nm}}} \tag{10.4}$$

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

```
q_ratio(sun.spct, Red("Smith10"), Far_red("Smith10"))

##  Red.Smith10: FarRed.Smith10(q:q)
##                          1.266704
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

Function `q_ratio` also accepts lists of wavebands, for both denominator and numerator arguments, and recycling takes place when needed. Calculation of the contribution of different colors to visible light, using ISO-standard definitions.

```
q_ratio(sun.spct, UVB(), list(UV(), VIS()))

##  UVB.ISO: UV.ISO.tr.lo(q:q)
##                 0.019369458
##       UVB.ISO: VIS.ISO(q:q)
##                 0.001541437
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

[4] In the original text photon fluence rate is used but it not clear whether photon irradiance was meant instead.

```
q_ratio(sun.spct,
        list(Red(), Green(), Blue()), VIS())

##    Red.ISO: VIS.ISO(q:q)  Green.ISO: VIS.ISO(q:q)
##                0.4150475                0.2025936
##   Blue.ISO: VIS.ISO(q:q)
##                0.1371157
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

or using a predefined list of wavebands:

```
q_ratio(sun.spct, VIS_bands(), VIS())

##  Purple.ISO: VIS.ISO(q:q)
##                0.15087813
##    Blue.ISO: VIS.ISO(q:q)
##                0.13711571
##   Green.ISO: VIS.ISO(q:q)
##                0.20259364
##  Yellow.ISO: VIS.ISO(q:q)
##                0.06106049
##  Orange.ISO: VIS.ISO(q:q)
##                0.05545498
##     Red.ISO: VIS.ISO(q:q)
##                0.41504754
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

Using spectral data stored in numeric vectors:

```
with(sun.spct,
     photon_ratio(w.length, s.e.irrad,  Red("Smith10"), Far_red("Smith10")))

## [1] 1.266704
```

10.11 Task: energy ratios

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

```
e_ratio(sun.spct, Red("Smith10"), Far_red("Smith10"))

##  Red.Smith10: FarRed.Smith10(e:e)
##                          1.401142
## attr(,"radiation.unit")
## [1] "e:e ratio"
```

other examples in section 10.10 above, can be easily edited to use `e_ratio` instead of `q_ratio`.

Using spectral data stored in vectors:

```
with(sun.spct,
     energy_ratio(w.length, s.e.irrad,
                  Red("Smith10"), Far_red("Smith10")))

## [1] 1.401142
```

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

10.12 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 $\mathrm{mol\,J^{-1}}$. In this case only one waveband definition is used to calculate the quotient:

$$\bar{q'} = \frac{Q_{\lambda_1<\lambda<\lambda_2}}{E_{\lambda_1<\lambda<\lambda_2}} \tag{10.5}$$

From this equation it follows that the value of the ratio will depend on the shape of the emission spectrum of the radiation source. For example, for PAR the R code is:

```
qe_ratio(sun.spct, PAR())

##    q:e( PAR)
## 4.547199e-06
## attr(,"radiation.unit")
## [1] "q:e ratio"
```

for obtaining the same quotient in $\mathrm{\mu mol\,J^{-1}}$ we just need to multiply by 1×10^6,

```
qe_ratio(sun.spct, PAR()) * 1e6

## q:e( PAR)
##  4.547199
## attr(,"radiation.unit")
## [1] "q:e ratio"
```

The seldom needed inverse ratio in $\mathrm{J\,mol^{-1}}$ can be calculated with function `eq_ratio`.

Both functions accept lists of wavebands, so several ratios can be calculated with a single function call:

```
qe_ratio(sun.spct, VIS_bands())

## q:e( Purple.ISO)   q:e( Blue.ISO)
##     3.433902e-06     3.968591e-06
##  q:e( Green.ISO) q:e( Yellow.ISO)
##     4.469290e-06     4.851392e-06
## q:e( Orange.ISO)    q:e( Red.ISO)
##     5.020950e-06     5.682783e-06
## attr(,"radiation.unit")
## [1] "q:e ratio"
```

The same ratios can be calculated for data stored in numeric vectors using function `photons_energy_ratio`:

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

## [1] 4.547199e-06
```

For obtaining the same quotient in $\mu mol\,J^{-1}$ from spectral data in $W\,m^{-2}\,nm^{-1}$ we just need to multiply by 1×10^6:

```
with(sun.spct,
     photons_energy_ratio(w.length, s.e.irrad, PAR())) * 1e6

## [1] 4.547199
```

10.13 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. When working with `source_spct` objects, the best way to achieve this is to combine the use of the functions `e_irrad` and `split_bands` already described above, for example,

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

##  range.400.500  range.500.600  range.600.700
##       69.69043       68.48950       58.45434
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

or

```
e_irrad(sun.spct, split_bands(PAR(), length.out=3))

##  range.400.500  range.500.600  range.600.700
##       69.69043       68.48950       58.45434
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

or

```
my_bands <- split_bands(PAR(), length.out=3)
e_irrad(sun.spct, my_bands)

##  range.400.500  range.500.600  range.600.700
##       69.69043       68.48950       58.45434
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

For the example immediately above, we can calculate relative values as

```
e_irrad(sun.spct, my_bands) / e_irrad(sun.spct, PAR())
```

```
##  range.400.500  range.500.600  range.600.700
##      0.3544165      0.3483091      0.2972744
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

or more efficiently as

```
irradiances <- e_irrad(sun.spct, my_bands)
irradiances / sum(irradiances)

##  range.400.500  range.500.600  range.600.700
##      0.3544165      0.3483091      0.2972744
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

The examples above use short names, the default, but longer names are also available,

```
e_irrad(sun.spct, split_bands(c(400, 500, 600, 700), short.names=FALSE))

##  range.400.500  range.500.600  range.600.700
##       69.69043       68.48950       58.45434
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"

e_irrad(sun.spct, split_bands(PAR(), short.names=FALSE, length.out=3))

##  range.400.500  range.500.600  range.600.700
##       69.69043       68.48950       58.45434
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

With spectral data stored in numeric vectors, we can use function `energy_irradiance` together with function `split_bands` or we can use the convenience function `split_energy_irradiance` to obtain to energy of each of the regions delimited by the values in nm supplied in a numeric vector:

```
with(sun.spct,
     split_energy_irradiance(w.length, s.e.irrad,
                             c(400, 500, 600, 700)))

## range.400.500 range.500.600 range.600.700
##      69.69043      68.48950      58.45434
```

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

```
with(sun.spct,
     split_energy_irradiance(w.length, s.e.irrad,
                             c(400, 500, 600, 700),
                             scale="relative"))
```

```
## range.400.500 range.500.600 range.600.700
##     0.3544165     0.3483091     0.2972744
```

or as percentages:

```
with(sun.spct,
     split_energy_irradiance(w.length, s.e.irrad,
                             c(400, 500, 600, 700),
                             scale="percent"))

## range.400.500 range.500.600 range.600.700
##      35.44165      34.83091      29.72744
```

If the 'limits' cover only a region of the spectral data, relative and percent values will be calculated with that region as a reference.

```
with(sun.spct,
     split_energy_irradiance(w.length, s.e.irrad,
                             c(400,500,600,700),
                             scale="percent"))

## range.400.500 range.500.600 range.600.700
##      35.44165      34.83091      29.72744
```

```
with(sun.spct,
     split_energy_irradiance(w.length, s.e.irrad,
                             c(400,500,600),
                             scale="percent"))

## range.400.500 range.500.600
##      50.43455      49.56545
```

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

```
with(sun.spct,
     split_energy_irradiance(w.length, s.e.irrad,
                             c(400, 700),
                             scale="percent"))

## range.400.700
##           100
```

In contrast, 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`:

```
with(sun.spct,
     split_energy_irradiance(w.length, s.e.irrad,
                             c(400, 700)))

## range.400.700
##      196.6343
```

10.14 Task: calculate the spectral overlap between two light sources

The first case assumes that we use the same photon irradiance for both sources, in this case two different types of LEDs.

The first step is to scale both spectra so that the photon irradiance is the same, in this case equal to one.

```
green.spct <- fscale(Norlux_G.spct,
                     range = c(400, 700),
                     f = "total",
                     unit.out = "photon")
blue.spct <- fscale(Norlux_B.spct,
                    range = c(400, 700),
                    f = "total",
                    unit.out = "photon")

overlapBG.s.q.irrad <- ifelse(green.spct$s.q.irrad < blue.spct$s.q.irrad,
                              green.spct$s.q.irrad,
                              blue.spct$s.q.irrad)

overlapBG.spct <- source_spct(w.length = blue.spct$w.length,
                              s.q.irrad = overlapBG.s.q.irrad)

integrate_spct(overlapBG.spct) /
    (integrate_spct(green.spct) + integrate_spct(blue.spct)) * 1e2

## q.irrad
## 3.93787
```

```
try(detach(package:lubridate))
try(detach(package:photobiologyLamps))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

11

Weighted and effective irradiance

11.1 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)
library(photobiologyWavebands)
library(photobiologyLamps)
library(lubridate)
```

11.2 Introduction

Weighted irradiance is usually reported in weighted energy units, but it is also possible to use weighted photon based units. In practice the R code to use is exactly the same as for unweighted irradiances, as all the information needed for applying weights is stored in the `waveband` object. An additional factor comes into play and it is the *normalization wavelength*, which is accepted as an argument by the predefined waveband creation functions that describe biological spectral weighting functions (BSWFs). The focus of this chapter is on the differences between calculations for weighted irradiances compared to those for un-weighted irradiances described in chapter 10. In particular it is important that you read sections **??**, 10.7, on the calculation of irradiances from spectral irradiances and sections 10.3, and 10.4 before reading the present chapter.

Most SWFs are defined using measured action spectra or spectra derived by combining different measured action spectra. As these spectra have been measured under different conditions, what is of interest is the shape of the curve as a function of wavelength, but not the absolute values. Because of this, SWFs are normalized to an action of one at an arbitrary wavelength. In many cases there is no consensus about the wavelength to use. Normalization is simple, it consists in dividing all action values along the curve by the action value at the selected normalization wavelengths.

Another complication is that it is not always clear if a given SWF definition is based on energy or photon units for the fluence rate or irradiances. In photobiology using photon units for expressing action spectra is the norm, but SWFs based on them have rather frequently been used as weights for spectral energy irradiance. Package 'photobiology' and the suite make this difference explicit, and uses the correct weights depending on the spectral data, as long as the `waveband` objects have been correctly defined. In the case of the definitions in package 'photobiologyWavebands', we have used, whenever possible the correct interpretation when described in the literature, or the common practice when information has been unavailable.

11.3 Task: specifying the normalization wavelength

Several constructors for SWF-based `waveband` objects are supplied. Most of them have parameters, in most cases with default arguments, so that different common uses and misuses in the literature can be reproduced. For example, function `GEN.G()` is predefined in package 'photobiologyWavebands' as a convenience function for Green's formulation of Caldwell's generalized plant action spectrum (GPAS) **Green198x**

```
e_irrad(sun.spct, GEN.G())

##  GEN.G.300.tr.lo
##        0.1028401
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

The code above uses the default normalization wavelength of 300 nm, which is almost universally used nowadays, but not the value used in the original publication (**Caldwell1973**). Any arbitrary wavelength (nm), within the range of the waveband is accepted as `norm` argument:

```
range(GEN.G())

## [1] 275.0 313.3

e_irrad(sun.spct, GEN.G(280))

##  GEN.G.280.tr.lo
##       0.02397171
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

11.4 Task: use of weighted wavebands

Please, consult the documentation of package 'photobiologyWavebands' for a list of predefined constructor functions for weighted wavebands. Here we will present just a few examples of their use. We usually think of weighted irradiances as being defined only by the weighting function, however, as mentioned above, in many cases different normalization wavelengths are in use, and the result of calculations depends very strongly on which wavelength is used for normalization. In a few cases different mathematical formulations are available for the 'same' SWF, and the differences among them can be also important. In such cases separate functions are provided for each formulation (e.g. `GEN.N` and `GEN.T` for Green's and Thimijan's formulations of Caldwell's GPAS).

```
GEN.G()
```

```
## GEN.G.300
## low (nm) 275
## high (nm) 313
## weighted SWF
## normalized at 300 nm

GEN.T()

## GEN.T.300
## low (nm) 275
## high (nm) 345
## weighted SWF
## normalized at 300 nm
```

We can use one of the predefined functions to create a new `waveband` object, which as any other R object can be assigned to a variable:

```
cie <- CIE()
cie

## CIE98.298
## low (nm) 250
## high (nm) 400
## weighted SWF
## normalized at 298 nm
```

As described in section 10.3, there are several methods for querying and printing `waveband` objects. The same functions described for un-weighted `waveband` objects can be used with any `waveband` object, including those based on SWFs.

11.5 Task: define wavebands that use weighting functions

In sections ?? and 7.8 we briefly introduced functions `waveband` and `new_waveband`, and here we describe their use in full detail. Most users are unlikely to frequently need to define new `waveband` objects as common SWFs are already defined in package 'photobiologyWavebands'.

Although the constructors are flexible, and can automatically handle both definitions based on action or response spectra in photon or energy units, some care is needed when performance is important.

When defining a new weighted `waveband`, we need to supply to the constructor more information than in the case on un-weighted wavebands. We start with a simple 'toy' example:

```
toy.wb <- waveband(c(400,700), weight="SWF",
                   SWF.e.fun=function(wl){(wl / 550)^2},
                   norm=550, SWF.norm=550,
                   wb.name="TOY")
toy.wb

## TOY
## low (nm) 400
## high (nm) 700
## weighted SWF
## normalized at 550 nm
```

where the first argument is the range of wavelengths included, `weight="SWF"` indicates that spectral weighting will be used, `SWF.e.fun=function(wl)wl * 2 / 550` supplies an 'anonymous' spectral weighting function based on energy units, `norm=550` indicates the default normalization wavelength to use in calculations, `SWF.norm=550` indicates the normalization wavelength of the output of the SWF, and `wb.name="TOY"` gives a name for the waveband.

In the example above the constructor generates automatically the SWF to use with spectral photon irradiance from the function supplied for spectral energy irradiance. The reverse is true if only an SWF for spectral photon irradiance is supplied. If both functions are supplied, they are used, but no test for their consistency is applied.

11.6 Task: calculate effective energy irradiance

We can use the `waveband` object defined above in calculations:

```
e_irrad(sun.spct, toy.wb)

##      TOY
## 196.9238
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

Just in the same way as we can use those created with the specific constructors, including using anonymous objects created on the fly:

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

##  CIE98.298.tr.lo
##       0.08181583
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

or lists of wavebands, such as

```
e_irrad(sun.spct, list(GEN.G(), GEN.T()))

##  GEN.G.300.tr.lo  GEN.T.300.tr.lo
##        0.1028401        0.1473621
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

or

```
e_irrad(sun.spct, list(GEN.G(280), GEN.G(300)))

##  GEN.G.280.tr.lo  GEN.G.300.tr.lo
##       0.02397171       0.10284005
```

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

Nothing prevents the user from defining his or her own `waveband` object constructors for new SWFs, and making this easy was an important goal in the design of the packages.

11.7 Task: calculate effective photon irradiance

All what is needed is to use function `q_irrad` instead of `e_irrad`. However, one should think carefully if such a calculation is what is needed, as in some research fields it is rarely used, even when from the theoretical point of view would be in most cases preferable.


```
q_irrad(sun.spct, GEN.G())

##  GEN.G.300.tr.lo
##     2.578989e-07
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

11.8 Task: calculate daily effective energy exposure

11.8.1 From spectral daily exposure

To calculate daily exposure values, if we have available spectral daily exposure (time-integrated spectral irradiance for a whole day) we need to apply the same code as used above, but using the spectral daily exposure instead of spectral irradiance as starting point:

```
e_irrad(sun.daily.spct, GEN.G())

##  GEN.G.300.tr.lo
##         2786.987
## attr(,"time.unit")
## [1] "day"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

the output from the code above is in units of $\mathrm{J\,m^{-2}\,d^{-1}}$, the code below returns the same result in the more common units of $\mathrm{kJ\,m^{-2}\,d^{-1}}$:

```
e_irrad(sun.daily.spct, GEN.G()) * 1e-3

##  GEN.G.300.tr.lo
##         2.786987
## attr(,"time.unit")
```

```
## [1] "day"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

by comparing these result to those for effective irradiances above, it can be seen that the `time.unit` attribute of the spectral data is copied to the result, allowing us to distinguish irradiance values (`time.unit="second"`) from daily exposure values (`time.unit="day"`).

11.8.2 From spectral irradiance

To calculate daily exposure values, from a known constant irradiance, we need to take into account the total length of exposure per day. This is equivalent to calculating fluence.

```
fluence(qpanel.uvb313.spct, GEN.G(),
        exposure.time = duration(6, "hours"))

##  GEN.G.300
##   41175.89
## attr(,"radiation.unit")
## [1] "energy fluence (J m-2)"
## attr(,"exposure.duration")
## [1] "21600s (~6 hours)"
```

the output from the code above is in units of $\mathrm{J\,m^{-2}\,d^{-1}}$, the code below returns the same result in the more common units of $\mathrm{kJ\,m^{-2}\,d^{-1}}$:

```
fluence(qpanel.uvb313.spct, GEN.G(),
        exposure.time = duration(6, "hours")) * 1e-3

##  GEN.G.300
##   41.17589
## attr(,"radiation.unit")
## [1] "energy fluence (J m-2)"
## attr(,"exposure.duration")
## [1] "21600s (~6 hours)"
```

by comparing these result to those for effective irradiances above, it can be seen that the `exposure.duration` supplied is copied to the result, allowing us to know the exposure has been.

```
try(detach(package:lubridate))
try(detach(package:photobiologyLamps))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

12

Transmission and reflection

12.1 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)
library(photobiologyWavebands)
library(photobiologyFilters)
library(photobiologyLEDs)
```

12.2 Introduction

In this chapter we explain how to do calculations related to the description of absorption and reflection of UV and VIS radiation.

12.3 Task: absorbance and transmittance

Transmittance is defined as:

$$\tau(\lambda) = \frac{I}{I_0} = \frac{E(\lambda)}{E_0(\lambda)} = \frac{Q(\lambda)}{Q_0(\lambda)} \tag{12.1}$$

Given this simple relation $\tau(\lambda)$ can be calculated as a division between two "source_spct" objects. This gives the correct answer, but as an object of class "source.scpt".

```
tau <- spc_above / spc_below
```

Absorptance is just $1 - \tau(\lambda)$, but should be distinguished from absorbance ($A(\lambda)$) which is measured on a logarithmic scale:

$$A(\lambda) = -\log_{10} \frac{I}{I_0} \tag{12.2}$$

In chemistry 10 is always used as the base of the logarithm, but in other contexts sometimes e is used as base.

Given the simple equation, $A(\lambda)$ can be also easily calculated using the operators for spectra. This gives the correct answer, but in an object of class "source.scpt".

The conversion between $\tau(\lambda)$ and $A(\lambda)$ is:

$$A(\lambda) = -\log_{10} \tau(\lambda) \tag{12.3}$$

which in S language is:

```
my_T2A <- function(x) {-log10(x)}
```

The conversion between $A(\lambda)$ and $\tau(\lambda)$ is:

$$\tau(\lambda) = 10^{-A(\lambda)} \tag{12.4}$$

which in S language is:

```
my_A2T <- function(x) {10^-x}
```

Instead of these functions, the package 'photobiology' defines generic functions and specialized functions, that can be used on numeric vectors and on `filter_spct` objects. The functions defined above could be directly applied to vectors but doing this on a column in a `filter_spct` is more cumbersome. As the spectra objects are data.tables, one can add a new column, say with transmittances to a copy of the filter data as is shown in the next section.

12.4 Task: spectral absorbance from spectral transmittance

Using `filter_spct` objects, the calculations become very simple.

```
my_gg400.spct <- schott.mspct$GG400
T2A(my_gg400.spct)

## Object: filter_spct [1,001 x 3]
## Wavelength range 200 to 5200 nm, step 1 to 50 nm
##
## # A tibble: 1,001 x 3
##   w.length   Tfr     A
## *    <dbl> <dbl> <dbl>
## 1      200 1e-05     5
## 2      201 1e-05     5
## 3      202 1e-05     5
## 4      203 1e-05     5
## # ... with 997 more rows

a.gg400.spct <- T2A(my_gg400.spct, action="replace")
```

As in addition to the `T2A` method for `filter_spct` there is a `T2A` method available for numeric vectors.

```
my_gg400.spct <- schott.mspct$GG400
my_gg400.spct$A <- T2A(my_gg400.spct$Tfr)
my_gg400.spct

## Object: filter_spct [1,001 x 3]
## Wavelength range 200 to 5200 nm, step 1 to 50 nm
##
## # A tibble: 1,001 x 3
##   w.length   Tfr     A
## *    <dbl> <dbl> <dbl>
## 1      200 1e-05     5
```

```
## 2      201 1e-05     5
## 3      202 1e-05     5
## 4      203 1e-05     5
## # ... with 997 more rows
```

or even on single numeric values:

```
T2A(0.001)

## [1] 3
```

12.5 Task: spectral transmittance from spectral absorbance

Please, see section 12.4 for more details in the description of the method `T2A` which does the opposite conversion than the method `A2T` needed for this task, but which works similarly.

```
A2T(a.gg400.spct)

## Object: filter_spct [1,001 x 3]
## Wavelength range 200 to 5200 nm, step 1 to 50 nm
##
## # A tibble: 1,001 x 3
##   w.length     A   Tfr
## *    <dbl> <dbl> <dbl>
## 1      200     5 1e-05
## 2      201     5 1e-05
## 3      202     5 1e-05
## 4      203     5 1e-05
## # ... with 997 more rows

A2T(a.gg400.spct, action="replace")

## Object: filter_spct [1,001 x 2]
## Wavelength range 200 to 5200 nm, step 1 to 50 nm
##
## # A tibble: 1,001 x 2
##   w.length   Tfr
## *    <dbl> <dbl>
## 1      200 1e-05
## 2      201 1e-05
## 3      202 1e-05
## 4      203 1e-05
## # ... with 997 more rows
```

12.6 Task: reflected or transmitted spectrum from spectral reflectance and spectral irradiance

When we multiply a `source_spct` by a `filter_spct` or by a `reflector_spct` we obtain as a result a new `source_spct`.

```
class(sun.spct)

## [1] "source_spct"  "generic_spct" "tbl_df"
## [4] "tbl"          "data.frame"

class(schott.mspct$GG400)

## [1] "filter_spct"  "generic_spct" "tbl_df"
## [4] "tbl"          "data.frame"
```

```
my_sun.spct <- sun.spct
my_gg400.spct <- schott.mspct$GG400
filtered_sun.spct <- sun.spct * schott.mspct$GG400
class(filtered_sun.spct)

## [1] "source_spct"  "generic_spct" "tbl_df"
## [4] "tbl"          "data.frame"

head(filtered_sun.spct)

## Object: source_spct [6 x 2]
## Wavelength range 280 to 282.76923 nm, step 0.07692308 to 0.9230769 nm
## Time unit 1s
##
## # A tibble: 6 x 2
##   w.length s.e.irrad
## *    <dbl>     <dbl>
## 1 280.0000         0
## 2 280.9231         0
## 3 281.0000         0
## 4 281.8462         0
## # ... with 2 more rows
```

The result of the calculation can be directly used as an argument, for example, when calculating irradiance.

```
q_irrad(sun.spct, UV()) * 1e6

##  UV.ISO.tr.lo
##      86.49506
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

q_irrad(my_sun.spct, UV()) * 1e6

##  UV.ISO.tr.lo
##      86.49506
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

q_irrad(filtered_sun.spct, UV()) * 1e6

##  UV.ISO.tr.lo
##      2.623568
```

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

q_irrad(sun.spct * schott.mspct$GG400, UV()) * 1e6

##  UV.ISO.tr.lo
##      2.623568
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

q_irrad(my_sun.spct * my_gg400.spct, UV()) * 1e6

##  UV.ISO.tr.lo
##      2.623568
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

```
q_irrad(my_sun.spct * my_gg400.spct) * 1e6

##    Total
## 1135.486
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

q_irrad(my_sun.spct * my_gg400.spct,
             new_waveband(min(sun.spct), max(sun.spct))) * 1e6

##  range.280.800
##       1135.486
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

Remember, that if we want to predict the output of a light source composed of different lamps or LEDs we can add the individual spectral irradiance, but using data measured from the target positions of each individual light source. If we want then to add the effect of a filter we must multiply by the filter transmittance.

```
my_luminaire <-
  (0.5 * Norlux_B.spct + Norlux_R.spct) *  plexiglas.mspct$Clear_0A000_XT
my_luminaire

## Object: source_spct [2,080 x 2]
## Wavelength range 250 to 900 nm, step 0.01 to 0.47 nm
## Time unit 1s
##
## # A tibble: 2,080 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
```

```
## 1   250.00         0
## 2   250.01         0
## 3   250.48         0
## 4   250.95         0
## # ... with 2,076 more rows

# equivalent
my_luminaire <-
  (Norlux_B.spct * 0.5 + Norlux_R.spct) *  plexiglas.mspct$Clear_0A000_XT
my_luminaire

## Object: source_spct [2,080 x 2]
## Wavelength range 250 to 900 nm, step 0.01 to 0.47 nm
## Time unit 1s
##
## # A tibble: 2,080 x 2
##   w.length s.e.irrad
##       <dbl>     <dbl>
## 1   250.00         0
## 2   250.01         0
## 3   250.48         0
## 4   250.95         0
## # ... with 2,076 more rows

q_ratio(my_luminaire,
            list(Red(), Blue(), Green()), PAR())

##    Red.ISO: PAR(q:q)   Blue.ISO: PAR(q:q)
##          0.816195602          0.146121825
##  Green.ISO: PAR(q:q)
##          0.003908976
## attr(,"radiation.unit")
## [1] "q:q ratio"

q_irrad(my_luminaire,
            list(PAR(), Red(), Blue(), Green())) *  1e6

##          PAR      Red.ISO     Blue.ISO
## 1.591314e-02 1.298824e-02 2.325257e-03
##    Green.ISO
## 6.220409e-05
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

12.7 Task: total spectral transmittance from internal spectral transmittance and spectral reflectance

12.8 Task: combined spectral transmittance of two or more filters

12.8.1 Ignoring reflectance

12.8.2 Considering reflectance

12.9 Task: light scattering media (natural waters, plant and animal tissues)

```
try(detach(package:photobiologyFilters))
try(detach(package:photobiologyLEDs))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

13

Astronomy

13.1 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)
library(lubridate)
library(ggplot2)
library(ggmap)

cache <- TRUE
```

13.2 Introduction

13.2.1 Time coordinates

This chapter deals with calculations that require times and/or dates as arguments. One could use R's built-in functions for POSIXct but package 'lubridate' makes working with dates and times, much easier. Package 'lubridate' defines functions for decoding dates represented as character strings, and for manipulating dates and doing calculations on dates. Each one of the different functions shown in the code chunk below can decode dates in different formats as long as the year, month and date order in the string agrees with the name of the function.

```
ymd("20140320")

## [1] "2014-03-20"

ymd("2014-03-20")

## [1] "2014-03-20"

ymd("14-03-20")

## [1] "2014-03-20"

ymd("2014-3-20")

## [1] "2014-03-20"

ymd("2014/3/20")

## [1] "2014-03-20"
```

```
dmy("20.03.2014")

## [1] "2014-03-20"

dmy("20032014")

## [1] "2014-03-20"

mdy("03202014")

## [1] "2014-03-20"
```

Similar functions including hours, minutes and seconds are defined by `lubridate` as well as functions for manipulating dates, and calculating durations with all the necessary and non-trivial corrections needed for leap years, summer time, and other idiosyncracies of the calendar system.

Times and dates are stored in R objects in Universal Time Coordinates (UTC), but the time zone (`tz`) used for input and output can vary widely. The UTC 'time zone' corresponds to the Greenwich meridian without any shifts due to daylight-saving time throughout the year. The time offset between local time and UTC can vary throughout the year due to day-light saving times—winter vs. summer time—, or accross years through changes in legislation—e.g. date when when daylight saving time starts and ends, or changes in the geographical borders between time zones, or a country adopting a different time zone. Different names and abbreviations are used, for the same time zones. Examples of time zones are EET or Eastern European Time, CET or Central European Time. Functions in package 'lubridate' are of help for getting around these conversions but one should be always very careful as many functions use as default the 'locale' and 'TZ' settings queried from the operating system as defaults. This means that data saved at a different geographic location or using a computer with wrong settings, or saving data using a remote (e.g. cloud) server located in a different time zone, can all result in misinterpretation of time data. Furthermore, the same R script may yield different output when run in a different time zone, unless time zone is explicitly passed as an argument. This problem does not only affect times, but also dates.

```
ymd("20140320") # no time zone set, Date object

## [1] "2014-03-20"

ymd("20140320", tz = "Europe/Helsinki") # Eastern Europe

## [1] "2014-03-20 EET"

ymd("20140320", tz = "America/Buenos_Aires") # Argentina

## [1] "2014-03-20 ART"

ymd("20140320", tz = "Asia/Tokyo") # Japan

## [1] "2014-03-20 JST"

# time set according to time zone
ymd_hm("20140320 00:00") # assumes local tz, POSIXct object

## [1] "2014-03-20 UTC"
```

```
ymd_hm("20140320 00:00", tz = "Europe/Helsinki") # central Europe

## [1] "2014-03-20 EET"

ymd_hm("20140320 00:00", tz = "America/Buenos_Aires") # Argentina

## [1] "2014-03-20 ART"

ymd_hm("20140320 00:00", tz = "Asia/Tokyo") # Central Australia

## [1] "2014-03-20 JST"
```

In the example above, the data are read using the supplied time zone, and printed back in a the same time zone. An example follows whose result depends on the local time zone where this file is run.

```
# this is just a date object, which ignores the time zone
ymd("20140320") # assumes local tz, POSIXct object

## [1] "2014-03-20"

with_tz(ymd("20140320"), tz = "America/Buenos_Aires")

## [1] "2014-03-20"

# this is a POSIXct date + time object
ymd_hm("20140320 00:00") # assumes local tz, POSIXct object

## [1] "2014-03-20 UTC"

with_tz(ymd_hm("20140320 00:00"), tz = "America/Buenos_Aires")

## [1] "2014-03-19 21:00:00 ART"

# current system time zone
Sys.timezone()

## [1] "UTC"
```

We should make explicit the time zones used for both input and output to avoid any ambiguities.

```
with_tz(ymd("20140320", tz = "America/Buenos_Aires"), tz = "Europe/London")

## [1] "2014-03-20 03:00:00 GMT"

with_tz(ymd("20140320", tz = "Asia/Tokyo"), tz = "America/Buenos_Aires")

## [1] "2014-03-19 12:00:00 ART"

with_tz(ymd_hm("20140320 00:00", tz = "America/Buenos_Aires"), tz = "Asia/Tokyo")

## [1] "2014-03-20 12:00:00 JST"

with_tz(ymd_hm("20140320 00:00", tz = "Asia/Tokyo"), tz = "America/Buenos_Aires")

## [1] "2014-03-19 12:00:00 ART"
```

13.2.2 Geographic coordinates

For astronomical calculations we also need as argument geographical coordinates. One can supply latitude and longitude values, acquired with a GPS instrument or read from a map. However, when the location is searchable through Google Maps, it is also possible to obtain the coordinates on-the-fly. A query can be run from within R using packages 'RgoogleMaps', or 'ggmap', as done here—of course this requires internet access. When inputting coordinate values manually, they should in degrees as numeric values (in other words the fractional part is given as part of floating point number in degrees, and not as separate integers representing minutes and seconds of degree). Latitudes N are given by positive numbers and and latitudes S by negative numbers. Longitudes W of Greenwich are given as positive numbers and longitudes E of Greenwich as negative numbers.

```
geocode("Helsinki")

##        lon      lat
## 1 24.93838 60.16986

geocode("Viikinkaari 1, 00790 Helsinki, Finland")

##        lon     lat
## 1 25.01673 60.2253
```

13.3 Task: calculating the length of the photoperiod

Functions `day_length` and `night_length` have same parameter signature. They are vectorised for the `date` parameter.

Calculating the length of the current day is easy. We use the Greenwich meridian, and 60 degrees in the Northern and Southern hemispheres. `today`.

```
day_length(today(), lat =  60, lon = 0)

## [1] 16.82001

day_length(today(), lat = -60, lon = 0)

## [1] 7.179545
```

In the case of daylength calculations the longitude is almost irrelevant, and defaults to zero degrees. As the date defaults to 'today' the code above can be simplified.

```
day_length(lat =  60)

## [1] 16.82001

day_length(lat = -60)

## [1] 7.179545
```

Function `geocode` from package 'ggmap' returns suitable values in a `data.frame` based on search term(s). The returned value is a data frame, which can be passed as

argument for parameter `geocode`. The use of Google search has some restrictions that you will need to check before any intense or commercial use of their service.

```
my.city <- geocode('helsinki')
my.city

##        lon      lat
## 1 24.93838 60.16986
```

We can calculate the photoperiod for the current day as

```
day_length(geocode = my.city)

## [1] 16.86375
```

Or if we give a date explicitly using functions from package 'lubridate'.

```
day_length(ymd("2015-06-09"),
           geocode = my.city)

## [1] 18.33724

day_length(dmy("9.6.2015"),
           geocode = my.city)

## [1] 18.33724
```

Or for several consecutive days by supplying a vector of dates as argument.

```
my.dates <- seq(ymd("2015-01-01"), ymd("2015-12-31"), by = "month")
day_length(my.dates, geocode = my.city)

##  [1]  5.631414  7.666748 10.198903 13.049334
##  [5] 15.725621 17.989206 18.415188 16.613254
##  [9] 13.966014 11.265202  8.456788  6.112162
```

Or to get the results as a data frame.

Default time zone of `ymd` is UTC or GMT, but one should set the same time zone as will be used for further calculations.

```
photoperiods.df <-
  data.frame(date = my.dates,
             photoperiod = day_length(my.dates, geocode = my.city))
```

The six lines at the top of the output are

```
head(photoperiods.df, 6)

##         date photoperiod
## 1 2015-01-01    5.631414
## 2 2015-02-01    7.666748
## 3 2015-03-01   10.198903
## 4 2015-04-01   13.049334
## 5 2015-05-01   15.725621
## 6 2015-06-01   17.989206
```

The complementary function `night_length` gives

```
night_length(ymd("2015-06-09"),
             geocode = my.city)

## [1] 5.662765
```

Using the functions as described above, 'measures' the photoperiod according to a boundary between day and night at a solar elevation angle equal to zero. An additional parameter of the functions, described in section 13.4, allows setting this twilight angle in degrees or by name according to different twilight angle definitions.

13.4 Task: Calculating times of sunrise, solar noon and sunset

Functions `sunrise_time`, `sunset_time`, and `noon_time` have the same parameter signature—take the same arguments—but the values they return differ.

Be also aware that for summer dates the times are expressed accordingly. In the examples below this can be recognized for example, by the time zone being reported as EEST instead of EET for Eastern Europe.

Both latitude and longitude can be supplied, but be aware that if the returned value is desired in the local time coordinates, the time zone should match the longitude.

```
sunrise_time(today(tz = "UTC"), lat = 60, lon = 0, tz = "UTC")

## [1] "2016-07-28 03:41:06 UTC"

sunrise_time(today(tz = "Europe/Helsinki"), lat = 60, lon = 25, tz = "Europe/Helsinki")

## [1] "2016-07-29 05:03:11 EEST"

sunrise_time(today(tz = "Europe/Helsinki"), lat = 60, lon = 25, tz = "UTC")

## [1] "2016-07-29 02:03:11 UTC"
```

The angle used in the twilight calculation can be supplied, either as the name of a standard definition, or as an angle in degrees (negative for sun positions below the horizon). Positive angles can be used when the time of sun occlusion behind a building, mountain, or other obstacle needs to be calculated.

```
sunrise_time(today(tzone = "Europe/Helsinki"),
             lat = 60, lon = 25, tz = "Europe/Helsinki",
             twilight = "civil")

## [1] "2016-07-29 03:51:30 EEST"

sunrise_time(today(tzone = "Europe/Helsinki"),
             lat = 60, lon = 25, tz = "Europe/Helsinki",
             twilight = -10)

## [1] "2016-07-29 02:37:12 EEST"

sunrise_time(today(tzone = "Europe/Helsinki"),
             lat = 60, lon = 25, tz = "Europe/Helsinki",
             twilight = +12)

## [1] "2016-07-29 06:52:56 EEST"
```

Default latitude is zero (the Equator), the default longitude is zero (Greenwich), and default time zone for the functions in the 'photobiology' package is `"UTC"`. The default for `date` is the current day in time zone UTC. Using defaults the code is simpler, but this is not a good approach for scripts.

```
sunrise_time(lat = 60)

## [1] "2016-07-28 03:41:06 UTC"
```

By default a POSIXct object is returned. This object described a date and time in UTC. It is portable and safe. However, if one needs the time of the day as numeric value, one can supply additional arguments.

```
sunrise_time(today(tzone = "Europe/Helsinki"),
             lat = 60, lon = 25, tz = "Europe/Helsinki",
             unit.out = "hour")

## [1] 5.053114

sunrise_time(today(tzone = "Europe/Helsinki"),
             lat = 60, lon = 25, tz = "Europe/Helsinki",
             unit.out =  "minute")

## [1] 303.1869

sunrise_time(today(tzone = "Europe/Helsinki"),
             lat = 60, lon = 25, tz = "Europe/Helsinki",
             unit.out = "second")

## [1] 18191.21
```

We can reuse the array of dates from section 13.3, and the coordinates of Joensuu, to calculate the time at sunrise through the year.

```
time_at_sunrise.df <-
  data.frame(date = my.dates,
             sunrise_at =
               sunrise_time(my.dates,
                            geocode = my.city,
                            tz = "Europe/Helsinki"))
```

The six lines at the top of the output are

```
head(time_at_sunrise.df, 6)

##         date          sunrise_at
## 1 2015-01-01 2015-01-01 09:34:49
## 2 2015-02-01 2015-02-01 08:44:10
## 3 2015-03-01 2015-03-01 07:27:16
## 4 2015-04-01 2015-04-01 06:53:29
## 5 2015-05-01 2015-05-01 05:26:27
## 6 2015-06-01 2015-06-01 04:18:56
```

The complementary functions `sunset_time` and `noon_time` take exactly the same arguments as `sunrise_time`, but `noon_time` ignores any argument supplied for `twilight`.

Box 13.1: Astronomical calculations of the sun position

Function `sun_angles`, which is a modified version of function `sunAngle` from package 'ode' is used to calculate the elevation of the sun at given time and geographical coordinates. To calculate the times corresponding to a given solar elevation, the algorithm first searches for the local solar noon by finding the maximal solar elevation, and then searches for sunrise in the first half of the day and for sunset in the second half local solar day. Sunset and sunrise are by default based on a solar elevation angle equal to zero. However, an argument can be passed to parameter `twilight` to set the angle according to different conventions—civil, nautical, astronomical—, by giving one or two values for the angles. Day and night durations are calculated as time durations between sunrise and sunset (the default) or dusk and dawn or some other angle. The algorithm currently used is valid for years 1950–2050.

```
sunrise_time(today(tz = "UTC"), lat = 60, lon = 0, tz = "UTC")

## [1] "2016-07-28 03:41:06 UTC"

sunset_time(today(tz = "UTC"), lat = 60, lon = 0, tz = "UTC")

## [1] "2016-07-28 20:30:18 UTC"

noon_time(today(tz = "UTC"), lat = 60, lon = 0, tz = "UTC")

## [1] "2016-07-28 12:06:14 UTC"
```

Function `day_night` returns a list with the different times with a single call. As other functions described in this chapter, `day_night` is vectorised for the `date` parameter.

```
day_night(today(tz = "UTC"), lat = 60, lon = 0, tz = "UTC")

## $day
## [1] "2016-07-28"
##
## $sunrise
## [1] "2016-07-28 03:41:06 UTC"
##
## $noon
## [1] "2016-07-28 12:06:14 UTC"
##
## $sunset
## [1] "2016-07-28 20:30:18 UTC"
##
## $daylength
## [1] 16.82001
##
## $nightlength
## [1] 7.17999
```

As in earlier examples, we use `geocode` to obtain the latitude and longitude of cities, although for precise calculations for large cities using a street address or at least a postal code in addition to the name of the city is preferable. The calculations

below are for Buenos Aires on two different dates, by use of the optional argument `tz` we request the results to be expressed in local time for Buenos Aires.

```
geocode_BA <- geocode("Buenos Aires")
day_night(ymd("2013-12-21"),
          geocode = geocode_BA,
          tz = "America/Buenos_Aires")

## $day
## [1] "2013-12-21"
##
## $sunrise
## [1] "2013-12-21 05:42:00 ART"
##
## $noon
## [1] "2013-12-21 12:51:46 ART"
##
## $sunset
## [1] "2013-12-21 20:01:32 ART"
##
## $daylength
## [1] 14.32535
##
## $nightlength
## [1] 9.674652
```

Or with `unit.out` set to `"hour"`

```
day_night(ymd("2013-12-21"),
          geocode = geocode_BA,
          tz = "America/Argentina/Buenos_Aires",
          unit.out = "hour")

## $day
## [1] "2013-12-21"
##
## $sunrise
## [1] 5.700227
##
## $noon
## [1] 12.86291
##
## $sunset
## [1] 20.02557
##
## $daylength
## [1] 14.32535
##
## $nightlength
## [1] 9.674652
```

Next, we calculate day length based on different definitions of twilight for Helsinki, at the equinox:

```
geocode_He <- geocode("Helsinki")
geocode_He

##        lon      lat
## 1 24.93838 60.16986
```

```
day_length(ymd("2013-09-21"),
           geocode = geocode_He)

## [1] 12.12726

day_length(ymd("2013-09-21"),
           geocode = geocode_He,
           twilight = "civil")

## [1] 13.74757

day_length(ymd("2013-09-21"),
           geocode = geocode_He,
           twilight = "nautical")

## [1] 15.43463

day_length(ymd("2013-09-21"),
           geocode = geocode_He,
           twilight = "astronomical")

## [1] 17.28464
```

Or for a given angle in degrees, which for example can be positive in the case of an obstacle like a building or mountain, instead of negative as used for twilight definitions. In the case of obstacles the angle will be different for morning and afternoon, and can be entered as a numeric vector of length two.

```
day_length(ymd("2013-09-21"),
           geocode = geocode_He,
           twilight = c(20, 0))

## [1] 9.252127
```

13.5 Task: calculating the position of the sun

Function `sun_angles` not only returns solar elevation, it returns all the angles defining the position of the sun. The time argument to `sun_angles` is internally converted to UTC (universal time coordinates, which is equal to GMT) time zone, so time defined for any time zone is valid input. The time zone used by default for the output can vary as described in page 134, so it is more reliable specify the time coordinates used for the output with parameter `tz`, using arguments valid for pacakge `lubridate` — which is used internally by package 'photobiology'.

```
geocode_Jo <- geocode("80100 Joensuu, Finland")
geocode_Jo

##        lon      lat
## 1 29.77829 62.62812

my_time <- ymd_hms("2014-05-29 18:00:00", tz="EET")
sun_angles(my_time,
           geocode = geocode_Jo)
```

```
## $time
## [1] "2014-05-29 18:00:00 EEST"
##
## $longitude
## [1] 29.77829
##
## $latitude
## [1] 62.62812
##
## $azimuth
## [1] 267.5851
##
## $elevation
## [1] 25.81094
##
## $diameter
## [1] 0.5260482
##
## $distance
## [1] 1.013595
```

If we do not supply a time as argument, `sun_angles` calculates the current position of the sun—or at the time indicated by the computer. In this case giving the position of the sun in the sky of Joensuu at the time this .PDF file was generated.


```
sun_angles(geocode = geocode_Jo)
```

```
## $time
## [1] "2016-07-28 22:17:04 UTC"
##
## $longitude
## [1] 29.77829
##
## $latitude
## [1] 62.62812
##
## $azimuth
## [1] 2.324311
##
## $elevation
## [1] -8.640557
##
## $diameter
## [1] 0.5251464
##
## $distance
## [1] 1.015336
```

13.6 Task: plotting sun elevation through a day

Function `sun_angles` described above is vectorised, so it is very easy to calculate the position of the sun throughout a day at a given location on Earth. The example here uses only solar elevation, plotted for Helsinki through the course of 23 June 2014. We first create a vector of times, using `seq` which can be used with dates in addition

to numbers. In the case of dates the argument passed to parameter `by` is specified as a string.

```
opts_chunk$set(opts_fig_wide_full)
```

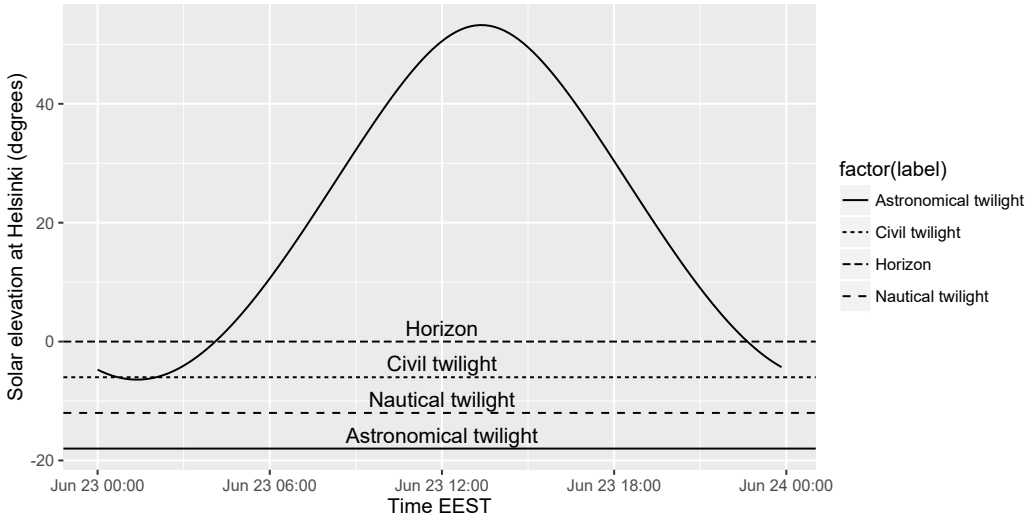
```
hours <- seq(from=ymd("2014-06-23", tz="EET"),
             by="10 min",
             length=24 * 6)
angles_He <- sun_angles(hours,
                        geocode = geocode_He)
sun_elev_hel <- data.frame(time_eet = hours,
                           elevation = angles_He$elevation,
                           azimuth = angles_He$azimuth)
head(sun_elev_hel)

##              time_eet elevation  azimuth
## 1 2014-06-23 00:00:00 -4.723353 341.1170
## 2 2014-06-23 00:10:00 -5.102431 343.3873
## 3 2014-06-23 00:20:00 -5.434211 345.6663
## 4 2014-06-23 00:30:00 -5.717998 347.9530
## 5 2014-06-23 00:40:00 -5.953188 350.2463
## 6 2014-06-23 00:50:00 -6.139276 352.5451
```

We also create an auxiliary data frame with data for plotting and labeling the different conventional definitions of *twilight*.

```
twilight <-
  data.frame(angle = c(0, -6, -12, -18),
             label = c("Horizon", "Civil twilight",
                       "Nautical twilight",
                       "Astronomical twilight"),
             time = rep(ymd_hms("2014-06-23 12:00:00",
                                tz="EET"),
                        4) )
```

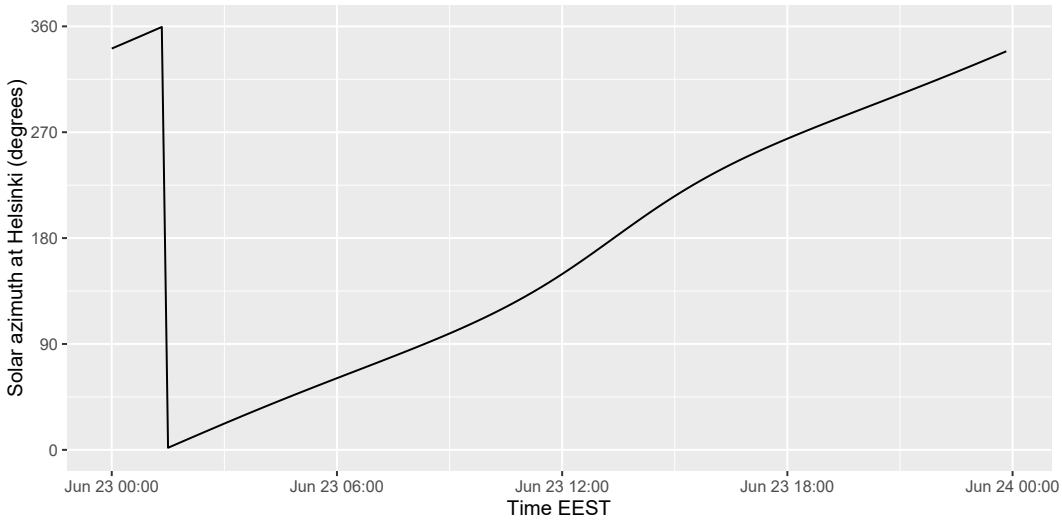
We draw a plot of solar elevations through a day, using the data frames created above.

```
ggplot(sun_elev_hel,
       aes(x = time_eet, y = elevation)) +
  geom_line() +
  geom_hline(data=twilight,
             aes(yintercept = angle, linetype=factor(label))) +
  annotate(geom="text",
           x=twilight$time, y=twilight$angle,
           label=twilight$label, vjust=-0.4, size=4) +
  labs(y = "Solar elevation at Helsinki (degrees)",
       x = "Time EEST")
```



We draw a plot of solar azimuths through a day, using the data frames created above.

```
ggplot(sun_elev_hel,
       aes(x = time_eet, y = azimuth)) +
  geom_line() +
  scale_y_continuous(breaks = c(0,90,180,270,360),
                     limits = c(0,360)) +
  labs(y = "Solar azimuth at Helsinki (degrees)",
       x = "Time EEST")
```



13.7 Task: plotting day length through the year

For this we first need to generate a sequence of dates. We use `seq` as in the previous section, but instead of supplying a length as argument we supply an ending time.

Instead of giving `by` in minutes as above, we now use days:

```
days <- seq(from=ymd("2014-01-01"), to=ymd("2014-12-31"),
            by="7 day")
```

We repeat the calculations for three locations at different latitudes, then row bind the data frames into a single data frame. Each individual data frame contains information to identify the sites:

```
geo_code_He <- geocode("Helsinki")
daylengths_hel <-
  data.frame(day = days,
             daylength = day_length(days,
                                    geocode = geo_code_He,
                                    tz = "EET"),
             location = "Helsinki")
```

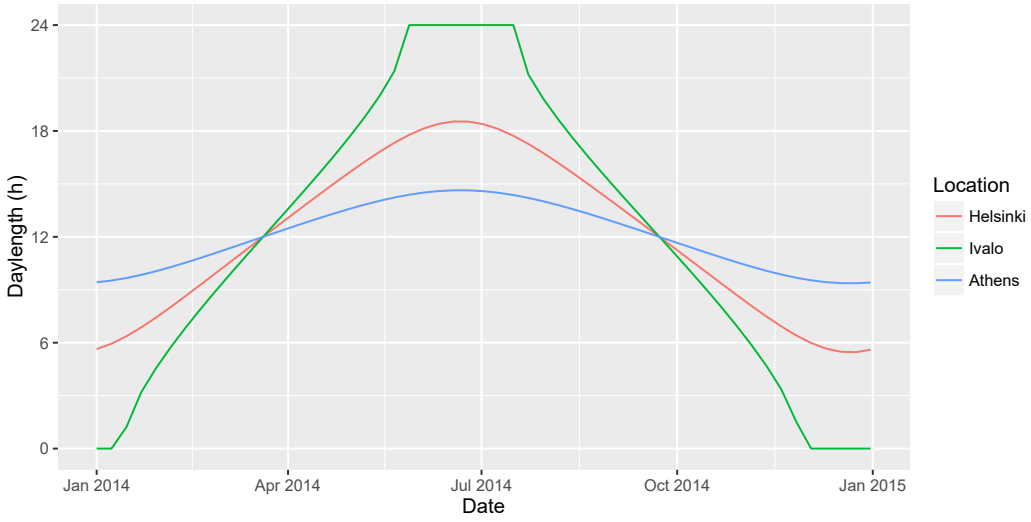
```
geo_code_Iv <- geocode("Ivalo")
daylengths_ivalo <-
  data.frame(day = days,
             daylength = day_length(days,
                                    geocode = geo_code_Iv,
                                    tz = "EET"),
             location = "Ivalo")
```

```
geo_code_At <- geocode("Athens, Greece")
daylengths_athens <-
  data.frame(day = days,
             daylength = day_length(days,
                                    geocode = geo_code_At,
                                    tz = "EET"),
             location = "Athens")
```

```
daylengths <- rbind(daylengths_hel,
                    daylengths_ivalo,
                    daylengths_athens)
```

Once we have the data available, plotting is simple:

```
ggplot(daylengths,
       aes(x = day, y = daylength, colour=factor(location))) +
  geom_line() +
  scale_y_continuous(breaks=c(0,6,12,18,24), limits=c(0,24)) +
  labs(x = "Date", y = "Daylength (h)", colour="Location")
```



13.8 Task: plotting local time at sunrise

For this we reuse `days` from the previous sections. We repeat the calculations for three locations at different latitudes, then row bind the data frames into a single data frame. Data frames contain information to identify the sites:

```
geo_code_He <- geocode("Helsinki")
sunrise_hel <-
  data.frame(day = days,
             sunrise = sunrise_time(days,
                                    geocode = geo_code_He,
                                    tz = "EET",
                                    unit.out = "hour"),
             location = "Helsinki")
```

```
geo_code_Iv <- geocode("Ivalo")
sunrise_ivalo <-
  data.frame(day = days,
             sunrise = sunrise_time(days,
                                    geocode = geo_code_Iv,
                                    tz = "EET",
                                    unit.out = "hour"),
             location = "Ivalo")
```

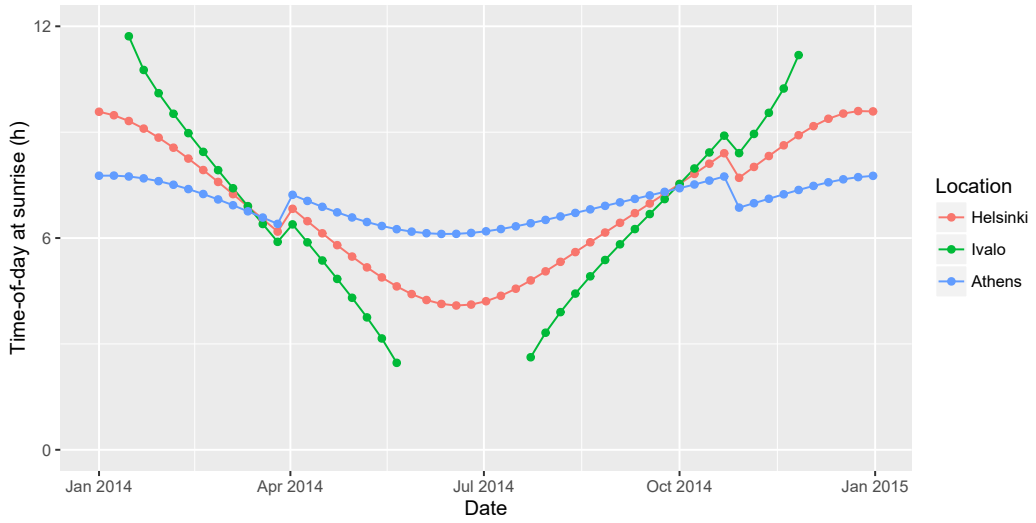
```
geo_code_At <- geocode("Athens, Greece")
sunrise_athens <-
  data.frame(day = days,
             sunrise = sunrise_time(days,
                                    geocode = geo_code_At,
                                    tz = "EET",
                                    unit.out = "hour"),
             location = "Athens")
```

The code below is quite complicated as we need to extract the times of day

```
sunrises <- rbind(sunrise_hel,
                  sunrise_ivalo,
                  sunrise_athens)
```

Once we have the data available, plotting is simple:

```
ggplot(sunrises,
       aes(x = day, y = sunrise, colour=factor(location))) +
  geom_line() + geom_point() +
  scale_y_continuous(breaks=c(0,6,12), limits=c(0,12)) +
  labs(x = "Date", y = "Time-of-day at sunrise (h)", colour="Location")

## Warning: Removed 7 rows containing missing values (geom_path).
## Warning: Removed 15 rows containing missing values
## (geom_point).
```



The breaks in the lines are the result of the changes between winter and summer time coordinates in the EET zone. The dots indicate the calculated values, once per week. Ivalo is above the northern polar circle, so in winter nights last for 24 h and in summer days last for 24 h.

By replacing `sunrise_time` by `sunset_time` in the code above and editing the axis label of the plot one can produce a similar plot of sunset times.

13.9 Task: plotting solar time at sunrise

```
try(detach(package:photobiology))
try(detach(package:lubridate))
try(detach(package:ggmap))
try(detach(package:ggplot2))
```

14

Colour

14.1 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)
```

14.2 Introduction

The calculation of equivalent colours and colour spaces is based on the number of photoreceptors and their spectral sensitivities. For humans it is normally accepted that there are three photoreceptors in the eyes, with maximum sensitivities in the red, green, and blue regions of the spectrum.

When calculating colours we can take either only the colour or both colour and apparent luminance. In our functions, in the first case one needs to provide as input 'chromaticity coordinates' (CC) and in the second case 'colour matching functions' (CMF). The suite includes data for humans, but the current implementation of the functions should be able to handle also calculations for other organisms with trichromic vision.

The functions allow calculation of simulated colour of light sources as R colour definitions. Three different functions are available, one for monochromatic light taking as argument wavelength values, and one for polychromatic light taking as argument spectral energy irradiances and the corresponding wave length values. The third function can be used to calculate a representative RGB colour for a band of the spectrum represented as a range of wavelengths, based on the assumption of a flat energy irradiance across this range.

By default CIE coordinates for *typical* human vision are used, but the functions have a parameter that can be used for supplying a different chromaticity definition. The range of wavelengths used in the calculations is that in the chromaticity data.

One use of these functions is to generate realistic colour for 'key' on plots of spectral data. Other uses are also possible, like simulating how different, different objects would look to a certain organism.

14.3 Task: calculating an RGB colour from a single wavelength

Function `w_length2rgb` must be used in this case. If a vector of wavelengths is supplied as argument, then a vector of `color` s, of the same length, is returned. Here are some examples of calculation of R color definitions for monochromatic light:

```
w_length2rgb(550) # green

## wl.550.nm
## "#00FF00"

w_length2rgb(630) # red

## wl.630.nm
## "#FF0000"

w_length2rgb(380) # UVA

## wl.380.nm
## "#000000"

w_length2rgb(750) # far red

## wl.750.nm
## "#000000"

w_length2rgb(c(550, 630, 380, 750)) # vectorized

## wl.550.nm wl.630.nm wl.380.nm wl.750.nm
## "#00FF00" "#FF0000" "#000000" "#000000"
```

14.4 Task: calculating an RGB colour for a range of wavelengths

Function `w_length_range2rgb` must be used in this case. This function expects as input a vector of two number, as returned by the function `range`. If a longer vector is supplied as argument, its range is used, with a warning. If a vector of lengths one is given as argument, then the same output as from function `w_length2rgb` is returned. This function assumes a flat energy spectral irradiance curve within the range. Some examples: Examples for wavelength ranges:

```
w_length_range2rgb(c(400,700))

## 400-700 nm
##  "#735B57"

w_length_range2rgb(400:700)

## Using only extreme wavelength values.

## 400-700 nm
##  "#735B57"

w_length_range2rgb(sun.spct$w.length)

## Using only extreme wavelength values.

## 280-800 nm
##  "#554340"

w_length_range2rgb(550)

## Calculating RGB values for monochromatic light.

## wl.550.nm
## "#00FF00"
```

14.5 Task: calculating an RGB colour for spectrum

Function `s_e_irrad2rgb` in contrast to those described above, when calculating the color takes into account the spectral irradiance.

Examples for spectra, in this case the solar spectrum:

```
with(sun.spct,
     s_e_irrad2rgb(w.length, s.e.irrad))

## [1] "#544F4B"

with(sun.spct,
     s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCMF2.spct))

## [1] "#544F4B"

with(sun.spct,
     s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCMF10.spct))

## [1] "#59534F"

with(sun.spct,
     s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCC2.spct))

## [1] "#B63C37"

with(sun.spct,
     s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCC10.spct))

## [1] "#BD3C33"
```

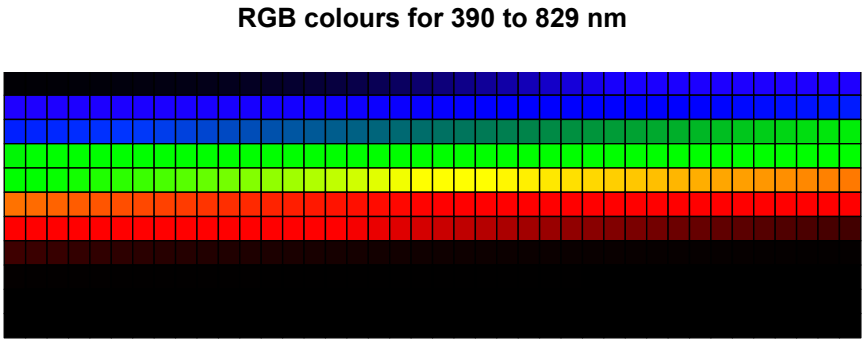
Except for the first example, we specificity the visual sensitivity data to use.

14.6 A sample of colours

Here we plot the RGB colours for the range covered by the CIE 2006 proposed standard calculated at each 1 nm step:

```
wl <- c(390, 829)

my.colors <- w_length2rgb(wl[1]:wl[2])

colCount <- 40 # number per row
rowCount <- trunc(length(my.colors) / colCount)

plot( c(1,colCount), c(0,rowCount), type="n",
      ylab="", xlab="",
      axes=FALSE, ylim=c(rowCount,0))
title(paste("RGB colours for",
            as.character(wl[1]), "to",
            as.character(wl[2]), "nm"))

for (j in 0:(rowCount-1))
{
  base <- j*colCount
  remaining <- length(my.colors) - base
```

```
  RowSize <-
    ifelse(remaining < colCount, remaining, colCount)
  rect((1:RowSize)-0.5, j-0.5, (1:RowSize)+0.5, j+0.5,
       border="black",
       col=my.colors[base + (1:RowSize)])
}
```




```
try(detach(package:photobiology))
```

15

Colour based indexes

15.1 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)
library(ggspectra)
library(photobiologyPlants)
library(hsdar)
```

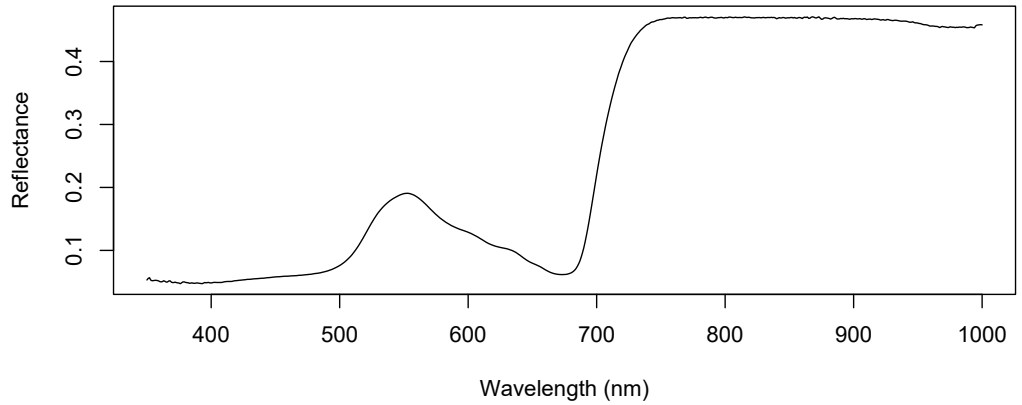
15.2 What are colour-based indexes?

15.3 Task: Calculation of the value of a known index from spectral data

We will start with a very well-known index used in remote sensing, Normalized Difference Vegetation Index (NDVI). We must be aware that an NDVI value calculated from spectral data on "first principles" may deviate from that obtained by means of non-spectral wide- or narrow-band sensors as used in used in satellites. Package 'hsdar' supplies spectral responses for satellites. So for remote sensing applications the use of this package is recommended.

We here demonstrate how to transfer a spectrum to 'hsdar', and one example of index calculation with this package. The 'hsdar' package can not only be used for individual spectra but also for hyperspectral images. Be aware, that this package seems to aim at data of rather low spectral resolution.

```
Solidago_hs.spct <- with(Solidago_upper_adax.spct, speclib(Rfr, w.length))
plot(Solidago_hs.spct)
ndvi <- vegindex(Solidago_hs.spct, "NDVI")
```



We now calculate a similar index by integrating reflectance for two wavebands,

```
normalized_diff_ind(Solidago_upper_adax.spct,
                    waveband(c(700, 1100)),
                    waveband(c(400, 700)),
                    reflectance)

## NDI  reflectance  [ 700.1100 ] - [ 400.700 ]
##                                    0.6355334
```

This returns a different value because, the wavebands are un-weighted, while weighting functions would be needed to reproduce NDVI.

15.4 Task: Estimation of an optimal index for discrimination

15.5 Task: Fitting a simple optimal index for prediction of a continuous variable

15.6 Task: PCA or PCoA applied to spectral data

15.7 Task: Working with spectral images

```
try(detach(package:hsdar))
try(detach(package:photobiologyPlants))
try(detach(package:ggspectra))
try(detach(package:photobiology))
```

16

Plotting spectra and colours

16.1 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(ggplot2)
library(scales)
library(ggtern)
library(gridExtra)
library(dplyr)
library(photobiology)
library(photobiologyFilters)
library(photobiologyWavebands)
library(photobiologyPlants)
library(photobiologyReflectors)
library(ggspectra)
```

16.2 Introduction to plotting spectra

We show in this chapter examples of how spectral data can be plotted. All the examples are done with package 'ggplot2', sometimes using in addition other packages. 'ggplot2' provides the most recent, but stable, type of plotting functionality in R, and is what we use here for most examples. Both `base` graphic functions, part of R itself and 'trellis' graphics provided by package 'lattice' are other popular alternatives. The new package 'ggvis' uses similar grammar as 'ggplot2' but drastically improves on functionality for interactive plots. Several of the functions used in this chapter are extensions to package 'ggplot2'[1]

How to depict a spectrum in a figure has to be thought in relation to what aspect of the information we want to highlight. A line plot of a spectrum with peaks and/or valleys labelled highlights the shape of the spectrum, while a spectrum plotted with the area below the curve filled highlights the total energy irradiance (or photon irradiance) for a given region of the spectrum. Adding a bar with the colours corresponding to the different wavelengths, facilitates the reading of the plot for people not familiar with the interpretation on wavelengths expressed in nanometres. Labeling regions of the spectrum with waveband names also facilitates the understanding of plotted

[1] 'ggplot2' is feature-frozen, in other words the user interface defined by the functions and their arguments will not change in future versions. Consequently it is a good basis for adding application-specific functionality through separate packages. 'ggplot2' uses the *grammar of graphics* for describing the plots. This grammar, because it is consistent, tends to be easier to understand, and makes it easier to design new functionality that uses extensions based on the same 'language grammar' as used by the original package.

spectral data. A basic line plot of spectral data can be easily done with 'ggplot2' or any of the other plotting functions in R. In this chapter we focus on how to add to basic line and dot plots all the 'fancy decorations' that can so much facilitate their reading and interpretation.

Towards the end of the chapter we give examples of plotting of RGB (red-green-blue) colours for human vision on a ternary plot, and show how to do a ternary plot for GBU (green-blue-ultraviolet) flower colours for honeybee vision using as reference the reflectance of a background.

If you are not familiar with 'ggplot2' and `ggtern` plotting, please read Appendix **??** on page **??** before continuing reading the present chapter.

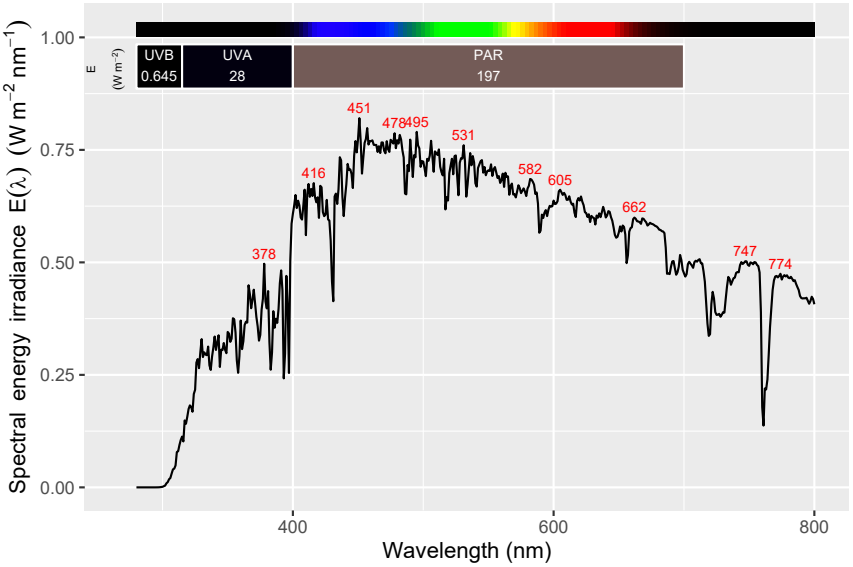
16.3 Using `plot()` methods with spectra

Package 'ggspectra' defines specializations of the generic `plot` function of R. These methods are available for all the different spectral object classes defined in package 'photobiology' except for `generic_spct`. They return a `ggplot` object, to which additional layers can be added if desired. An example of it simplest use follows in the next task. As all the spectral objects have spectral quantities expressed in known units, and an attribute indicating the time unit, the axis labels are produced automatically. If summaries are added, the units in their labels are also produced automatically. The plots produced can be to some extent tailored through options or by adding or replacing `ggplot` layers, the intention is for these methods to be a total that is simple, but that caters for the majority of the most frequent tasks.

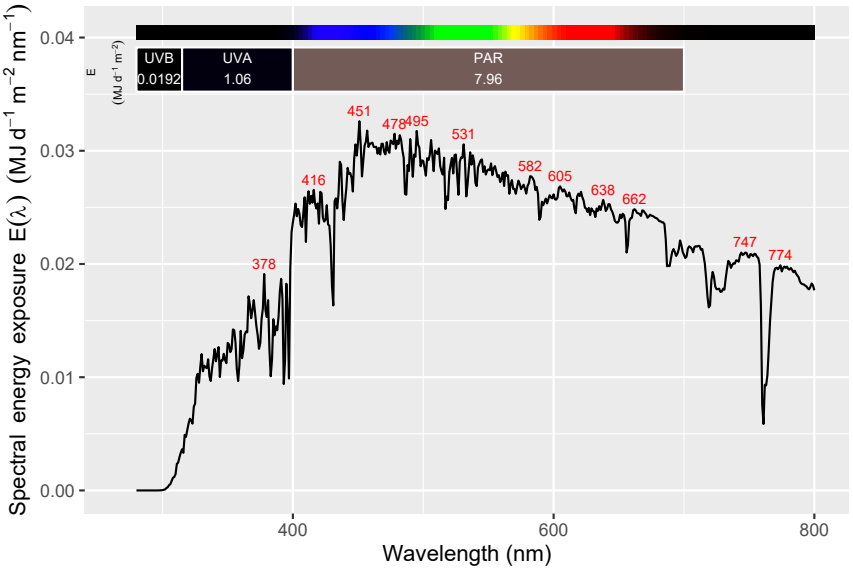
16.3.1 Task: plotting of `source_spct` objects

The defaults arguments cater the exploratory plotting of spectra, returning a plot that is heavily annotated, and using the most common units of expression. The two plots that follow show spectral irradiance, and spectral daily exposure, respectively. The objects plotted contain meta data that informs the time unit, so applying the same `plot` method, yields two plots with different units in the y-axis label.

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

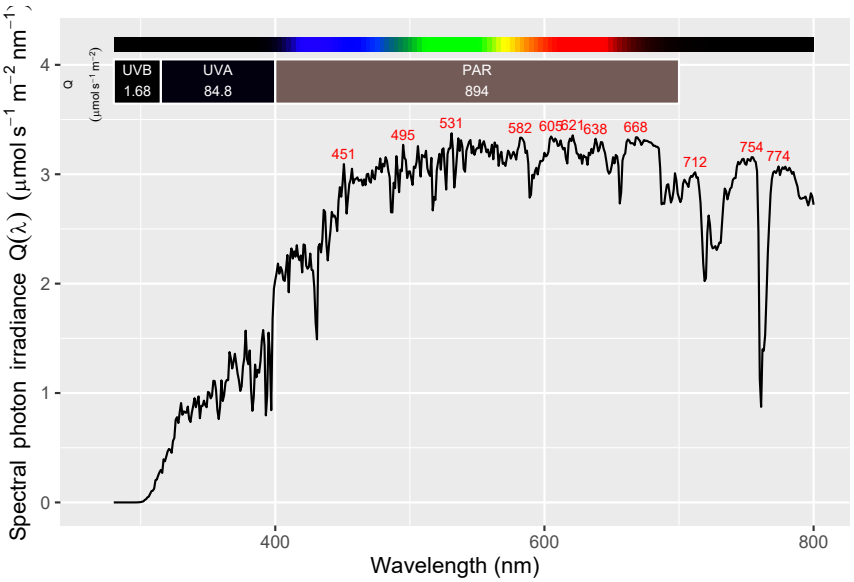



```
plot(sun.daily.spct)
```



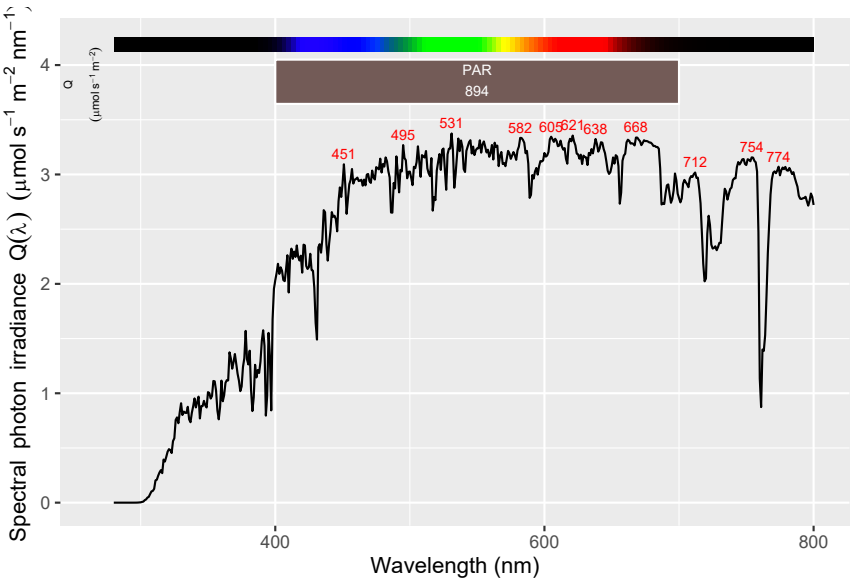
The parameter `unit` can be set to `"photon"` to obtain a plot depicting spectral photon irradiance. This works irrespective of whether the `source_spct` object contains spectral data expressed in photon or energy units—data are converted as needed.

```
plot(sun.spct, unit.out = "photon")
```

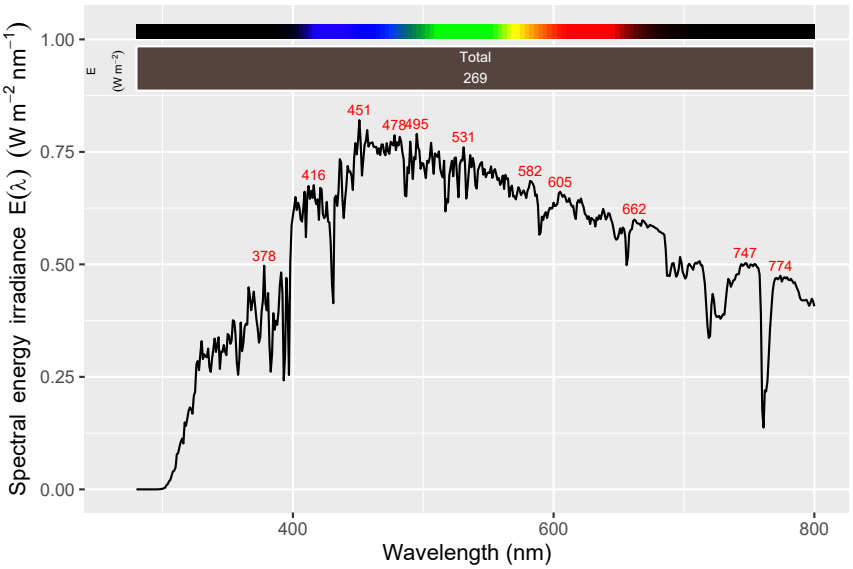


A list of wave bands, or a single wave band, to be used for annotation can be supplied through the `bands` parameter. A `NULL` waveband results in no waveband labels, while the next example shows how to obtain the total irradiance.

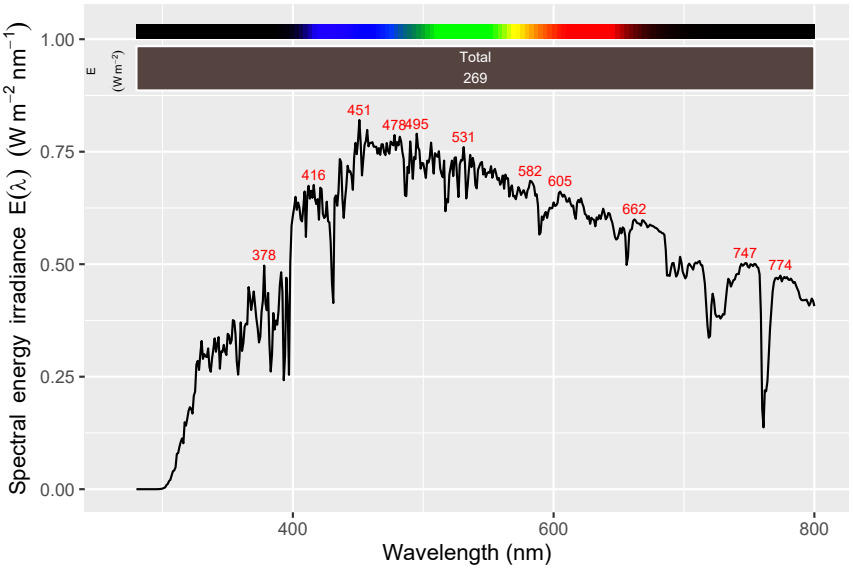
```
plot(sun.spct, w.band = PAR(), unit.out = "photon")
```




```
plot(sun.spct, w.band = NULL)
```

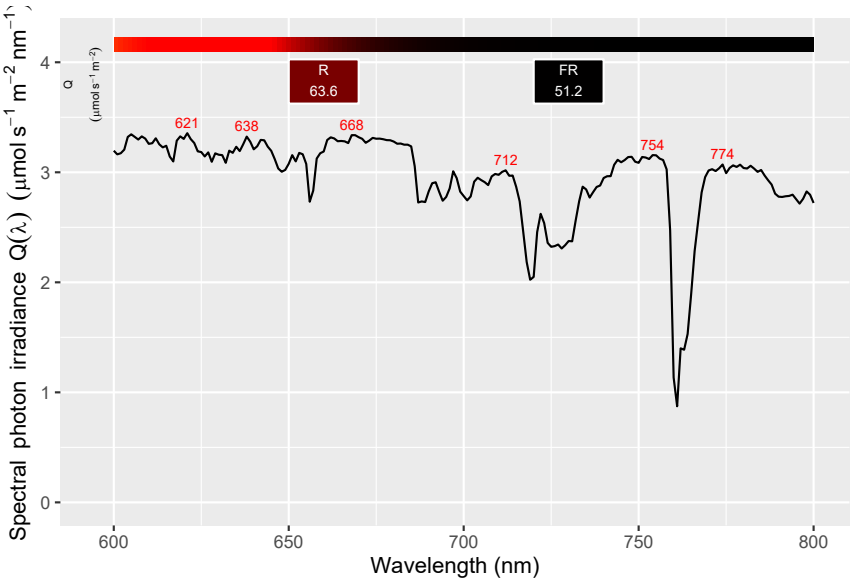



```
plot(sun.spct, w.band = waveband(sun.spct))
```



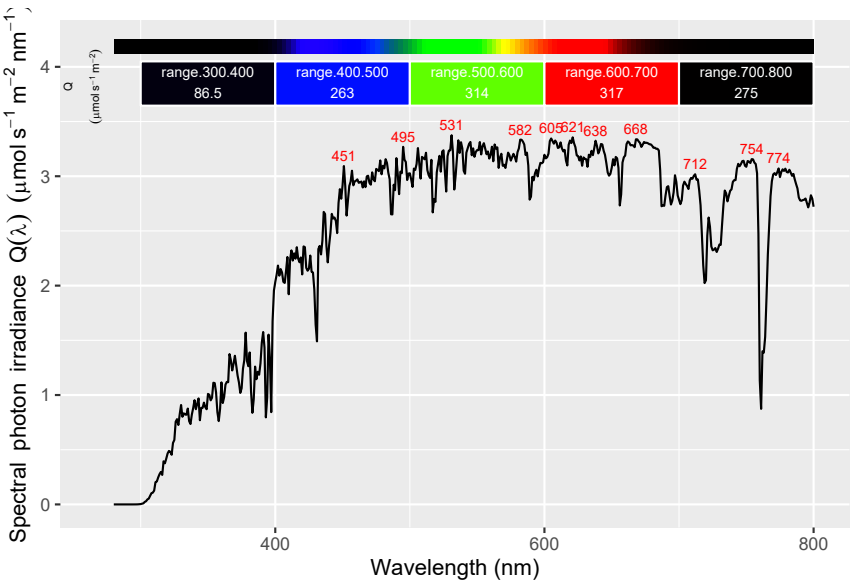
Of course the arguments to these parameters can be supplied in different combinations, and combined with other functions as needed. This last example shows how to plot using photon-based units, selecting only a specific region of the spectrum, annotated with the red and far-red photon irradiances, using Prof. Harry Smith's definitions for these two wavebands using 20-nm wide bands.

```
plot(trim_wl(sun.spct, waveband(c(600,800))),
     w.band = list(Red("Smith20"), Far_red("Smith20")), unit.out = "photon")
```

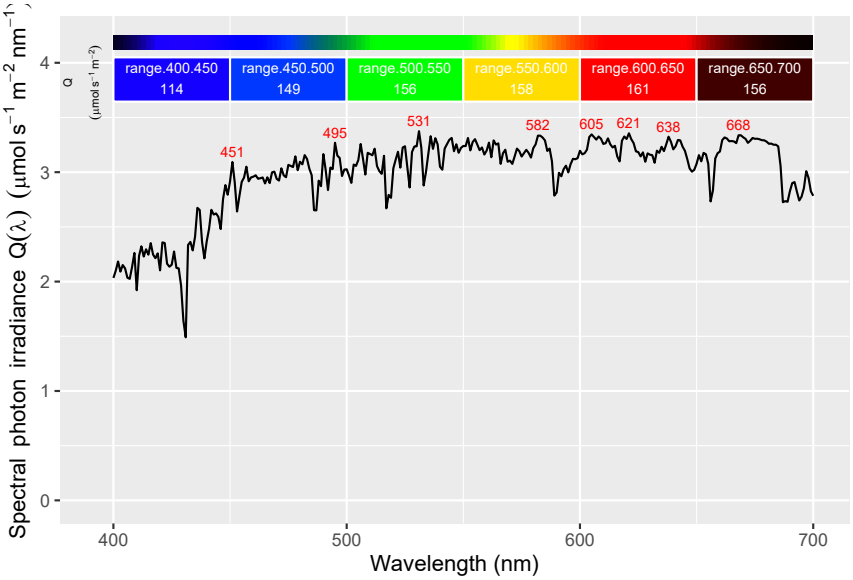


The next two examples show how to annotate an irradiance spectrum plot by equal sized wavebands.

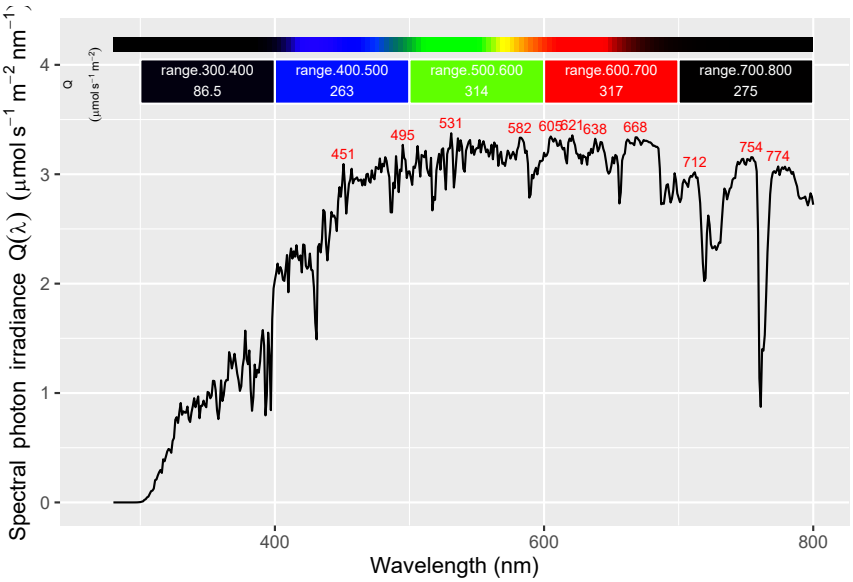
```
plot(sun.spct,
     w.band = split_bands(c(300,800), length.out = 5), unit.out = "photon")
```




```
plot(trim_wl(sun.spct, PAR()),
     w.band=split_bands(PAR(), length.out = 6), unit.out = "photon")
```

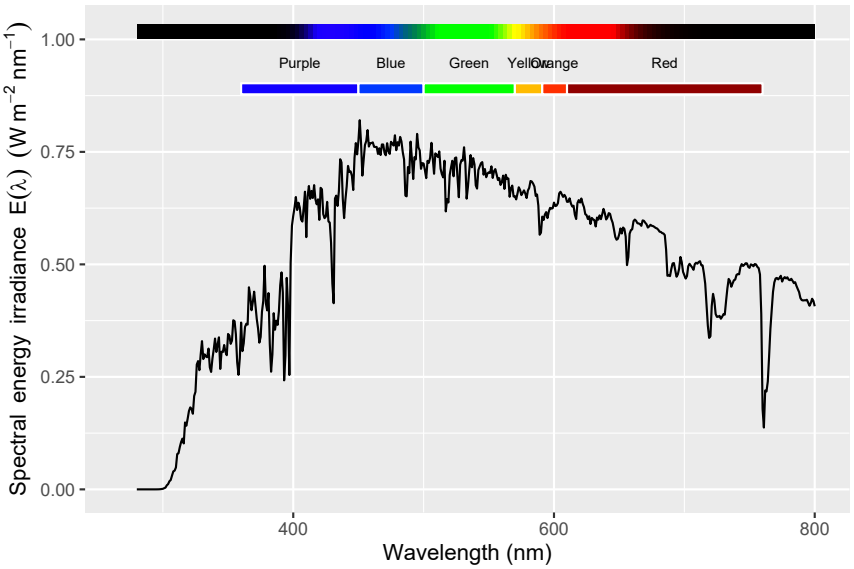



```
plot(sun.spct,
     w.band = split_bands(c(300,800), length.out = 5), unit.out = "photon")
```



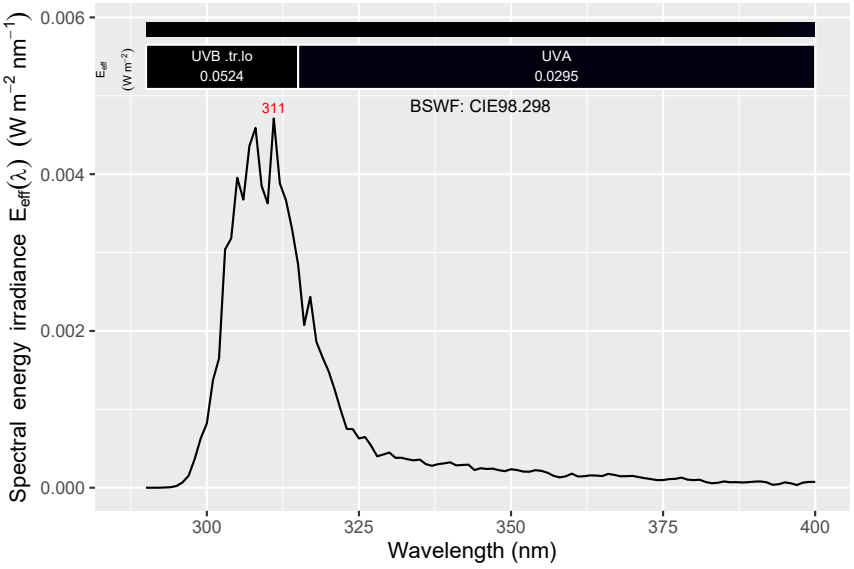
Which annotations are included, depends on the argument supplied, as exemplified below.

```
plot(sun.spct,
     annotations = c("color.guide","segments","labels"),
     w.band = VIS_bands("ISO"))
```

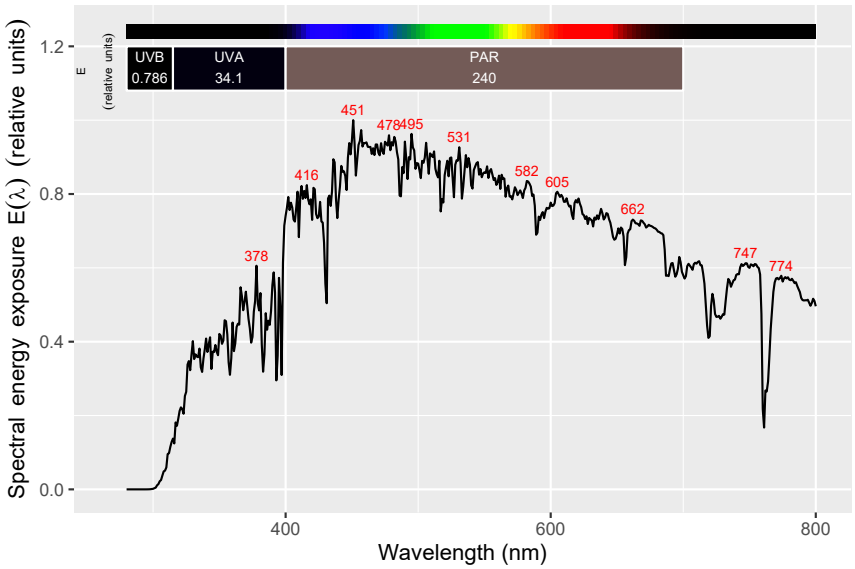


There are additional meta-data values stored in `source_spct` objects related to re-scaling, normalization and weighting of the spectral data. These all affect axis labels, and in the case of weighting, the name of the spectral weighting function is added to the plot as an annotation. The following examples exemplify some of these, plus the use of `range` to limit the range of wavelengths included in the plot.

```
plot(sun.spct * CIE(), range = c(290,400))
```




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

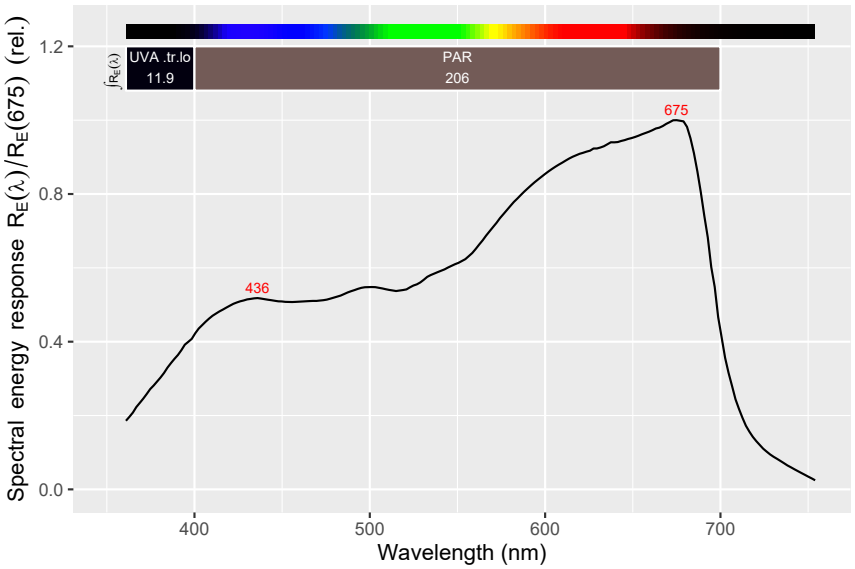


As the current implementation uses `ggplot` 'statistic's, waveband irradiance annotations respect global aesthetics and facets. If used for simultaneous plotting in the same panel of several spectra (stored *longitudinally* in a single R object), then a summary annotation should not be used as the values would be overplotted and ambiguous.

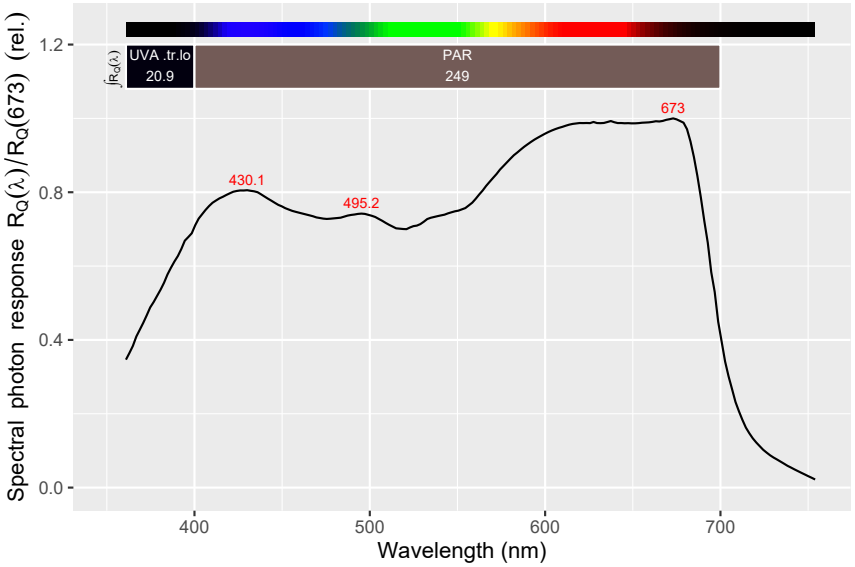
16.3.2 Task: plotting of `response_spct` objects

The defaults arguments cater the exploratory plotting of spectra, returning a plot that is heavily annotated. The two plots that follow show spectral response, expressed on an energy or photon basis. We use as example the action spectrum of photosynthesis in leaves.

```
plot(McCree_Oat.spct)
```




```
plot(McCree_Oat.spct, unit.out = "photon")
```



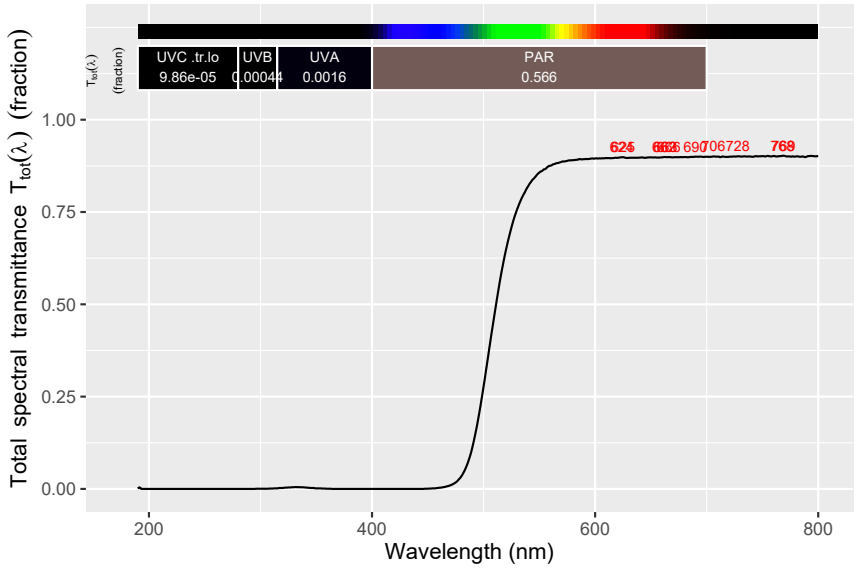
For details on how to modify the wavebands used for labels and summaries, and customization of annotations, please see the previous section 16.3.1 on page 156. As for other `plot` methods described in this chapter normalization and scaling metadata are reflected in the plot axis-labels.

16.3.3 Task: plotting of `filter_spct` objects

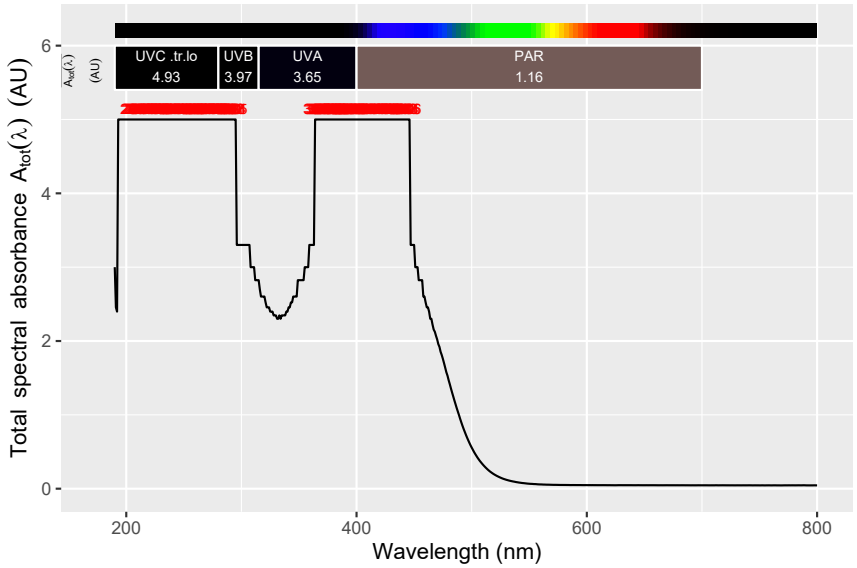
The defaults arguments cater the exploratory plotting of spectra, returning a plot that is heavily annotated, and using the most common units of expression. The three

plots that follow show spectral transmittance, spectral absorptance and spectral absorbance, respectively. The objects plotted contain meta data that informs wether transmittance is expressed as *internal* or *total*, so applying the same `plot` method, will produce plots with different units in the y-axis label in these two cases. The difference between internal and total transmittance is explained in section **??**.

```
plot(yellow_gel.spct)
```



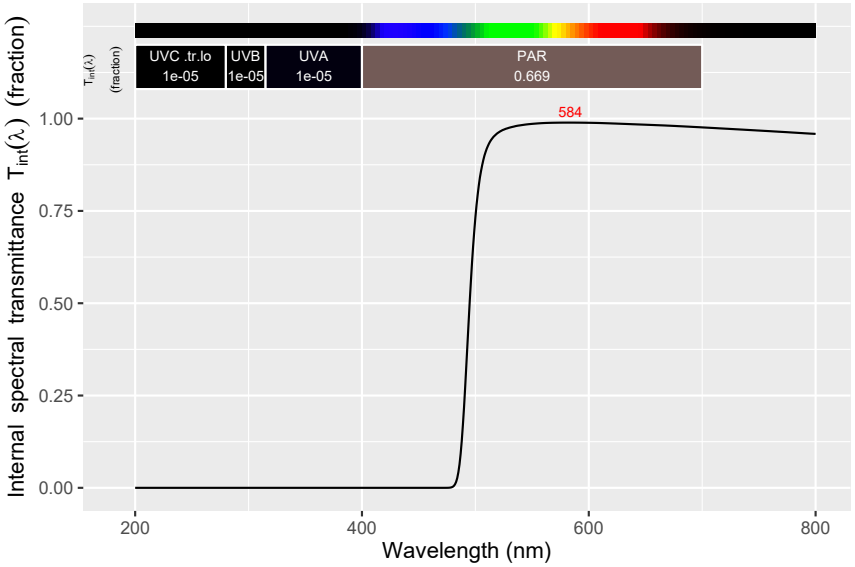

```
plot(yellow_gel.spct, plot.qty = "absorbance")
```



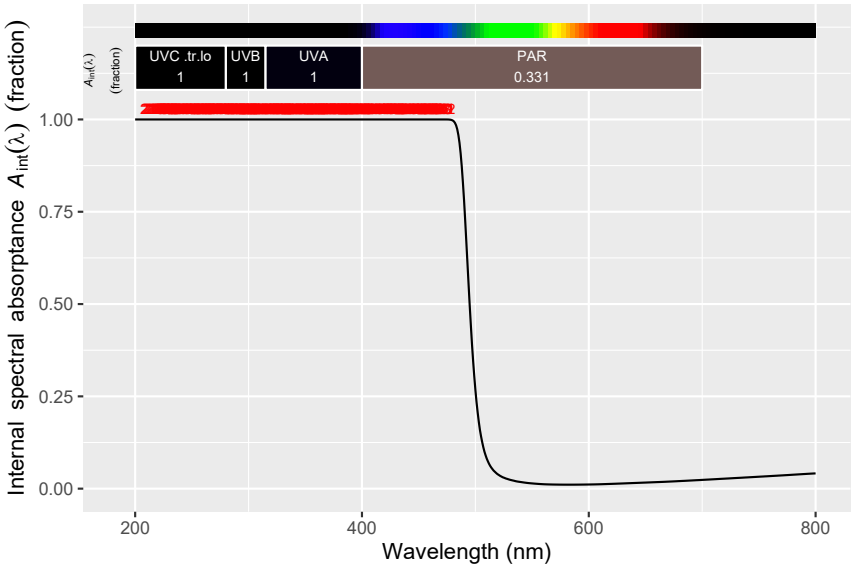
Beware that *absorptance* being the complement to *internal transmittance* can be calculated only from transmittance alone if it is expressed as internal. If total transmittance is available, then reflectance must be also known before absorptance can be

calcaluated. For this reason we use different spectral data for this example. We also illustrate how we can force the range of wavelengths included in the plot to match the range of another spectral object.

```
plot(schott.mspct$GG495, range = yellow_gel.spct)
```

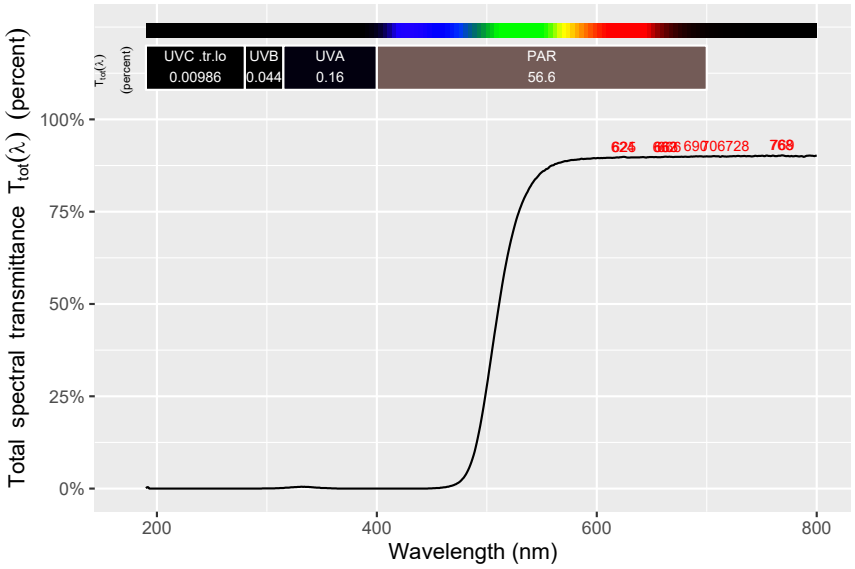



```
plot(schott.mspct$GG495, plot.qty = "absorptance",
     range = yellow_gel.spct)
```

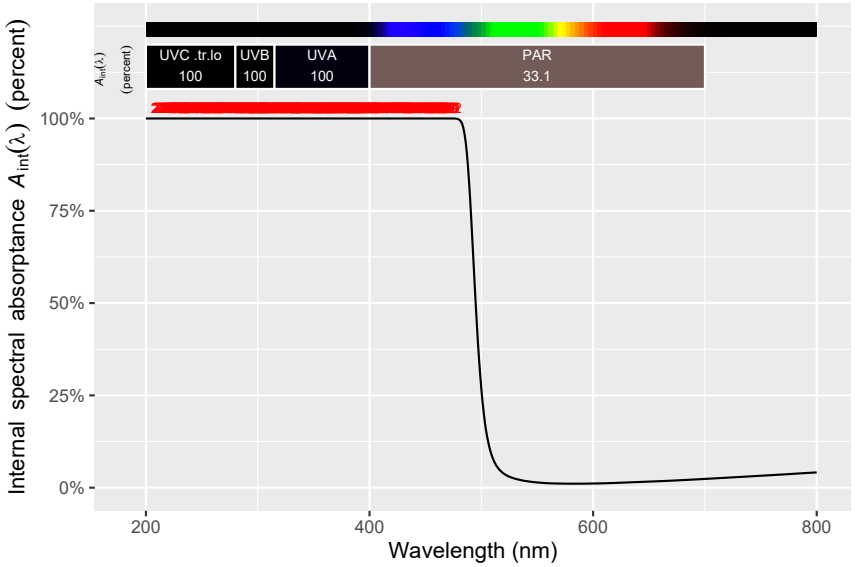


By default transmittance and absorptance are expressed as fractions of one. However, plotting of values expressed as percentages is also possible.

```
plot(yellow_gel.spct, pc.out = TRUE)
```




```
plot(schott.mspct$GG495, plot.qty = "absorptance",
     pc.out = TRUE, range = yellow_gel.spct)
```

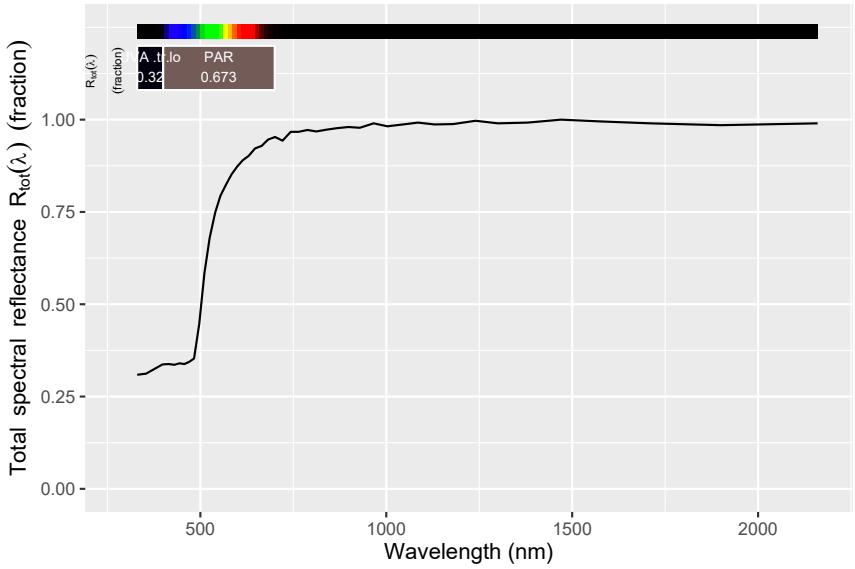


For details on how to modify the wavebands used for labels and summaries, and customization of annotations, please see the previous section 16.3.1 on page 156.

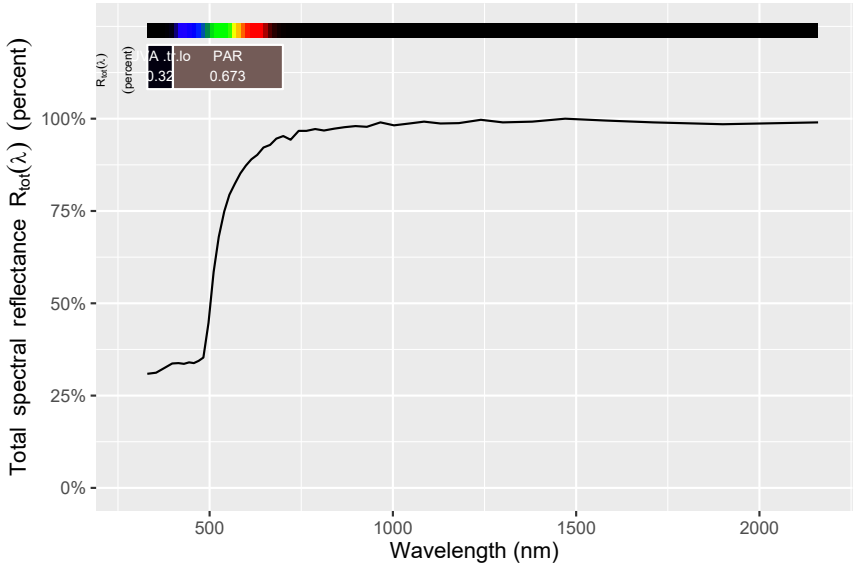
16.3.4 Task: plotting of `reflector_spct` objects

At the moment, the only `plot.qty` supported is *reflectance*.

```
plot(gold.spct)
```




```
plot(gold.spct, pc.out = TRUE)
```



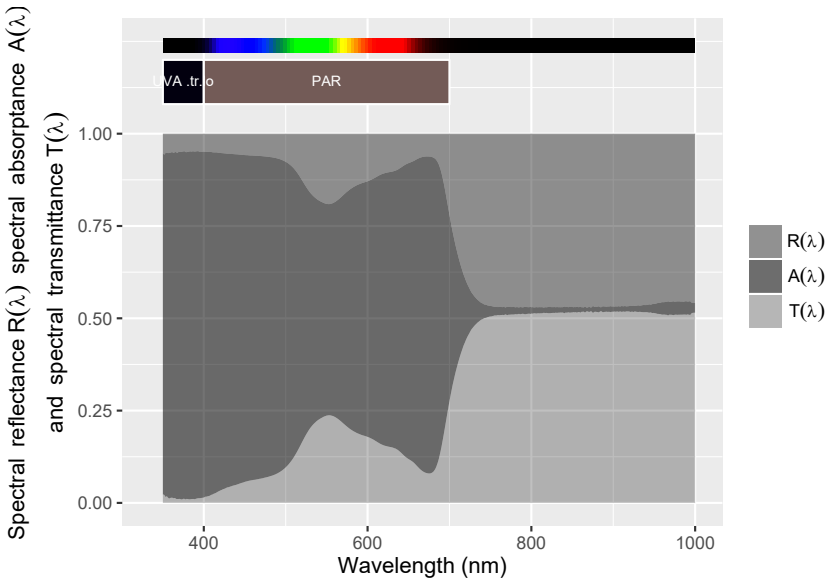
For details on how to modify the wavebands used for labels and summaries, and customization of annotations, please see the previous section 16.3.1 on page 156.

16.3.5 Task: plotting of `object_spct` objects

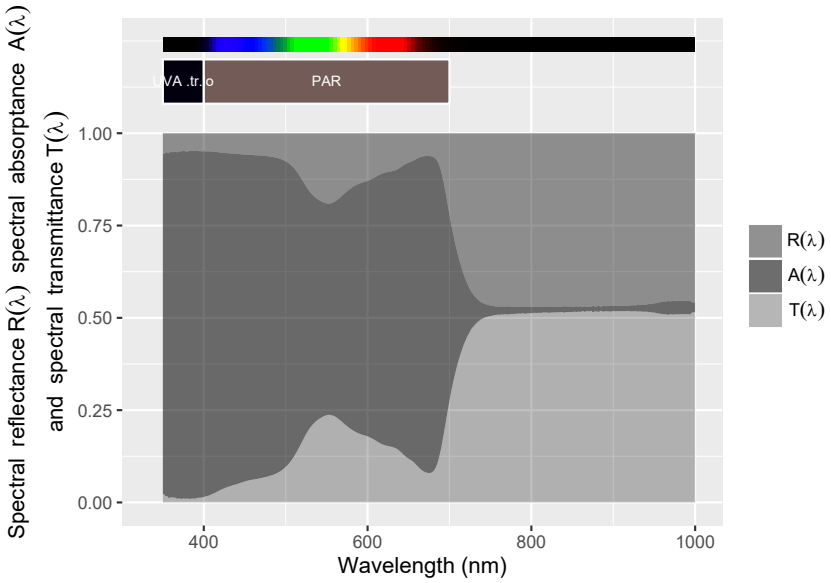
We will use as example the spectral properties of a plant leaf. This method is the most flexible with respect to the quantity plotted, as `object_spct` objects contain

more than one spectral quantity, and as $R + A + T = 1$, the three quantities are always available for plotting. By default, all three are plotted.

```
plot(Solidago_upper_adax.spct)
```

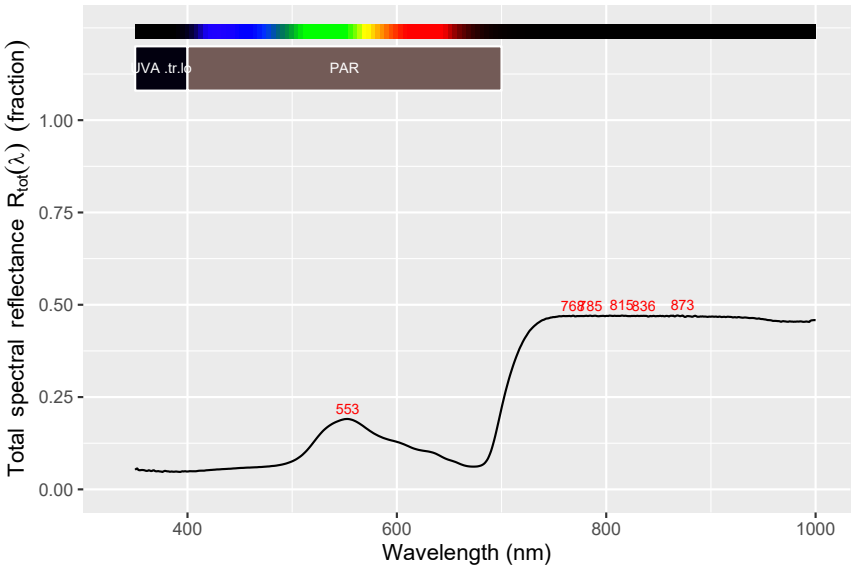



```
plot(Solidago_upper_adax.spct, plot.qty = "all")
```

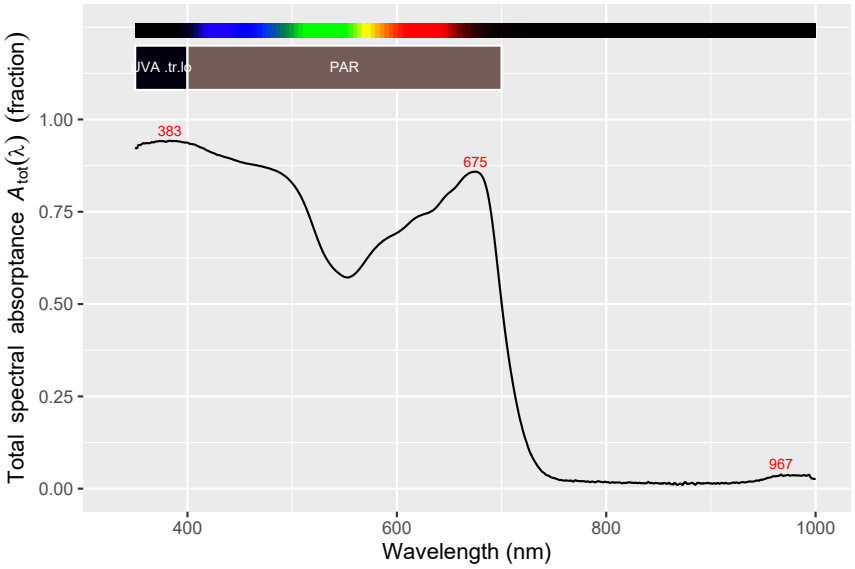


However, they can be plotted individually, as well as absorbance.

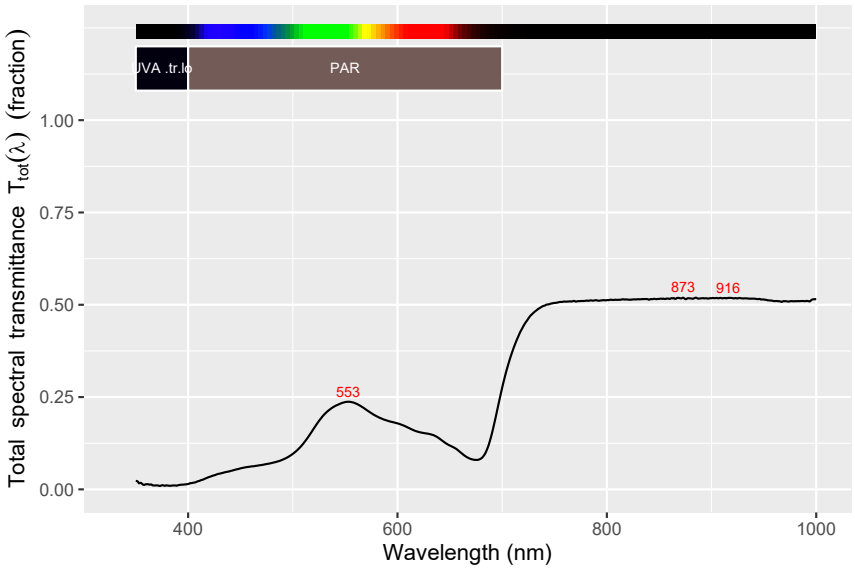
```
plot(Solidago_upper_adax.spct, plot.qty = "reflectance")
```



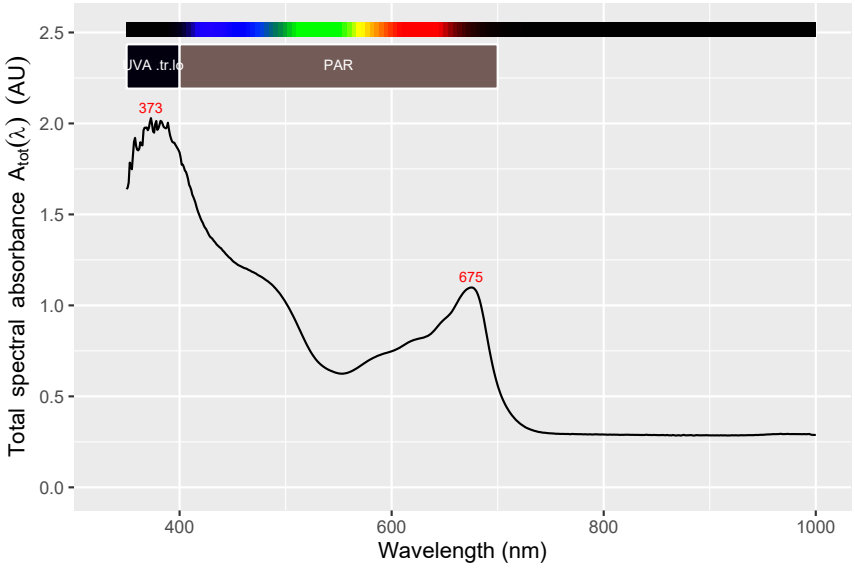

```
plot(Solidago_upper_adax.spct, plot.qty = "absorptance")
```




```
plot(Solidago_upper_adax.spct, plot.qty = "transmittance")
```

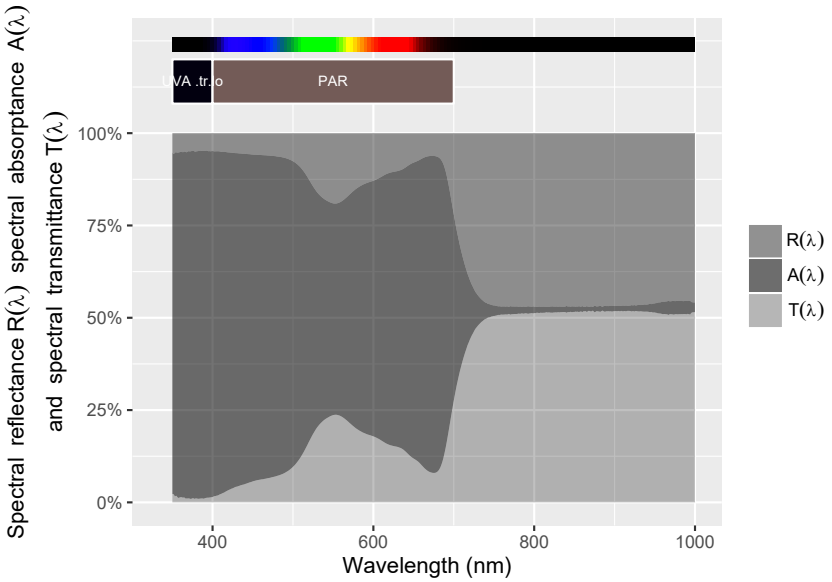



```
plot(Solidago_upper_adax.spct, plot.qty = "absorbance")
```



As for `filter_spct` and `reflector_spct` quantities can be plotted as percentages. We give only one example here.

```
plot(Solidago_upper_adax.spct, pc.out = TRUE)
```



For details on how to modify the wavebands used for labels and summaries, and customization of annotations, please see the previous section 16.3.1 on page 156.

16.4 Plotting spectra with 'ggplot2'

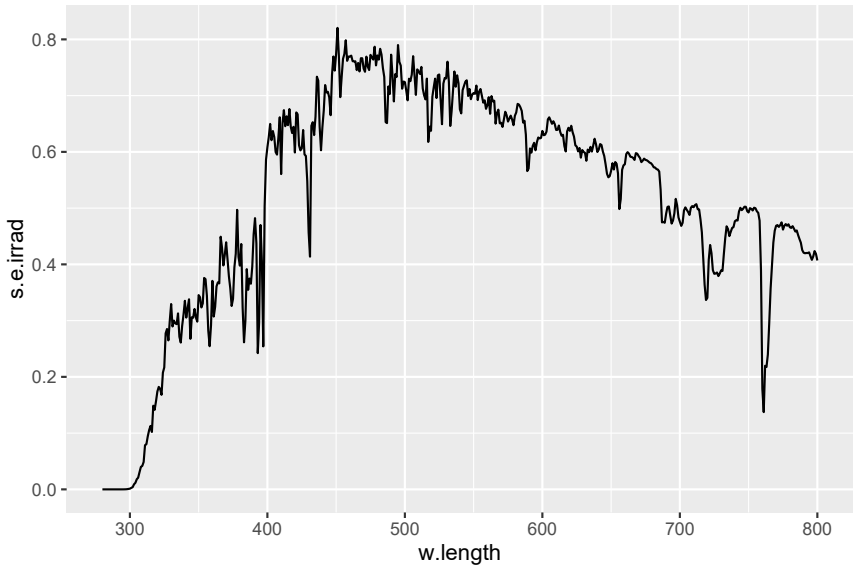
Package 'ggspectra' not only provides simple to use `plot` methods, but also 'building block' that simplify the construction of custom plots of spectral data with functions from package 'ggplot2'. In this section we give examples of plotting tasks carried out using this more flexible approach. In this chapter's examples we will exploit the power of the grammar of graphics to build figures piece by piece, reusing some of the 'pieces' or groups of 'pieces' several times to highlight the flexibility of this approach. We also exemplify the 'philosophy' of defining everything that needs to be consistent across figures only once. In this section we use a `source_spct` object, `sun.spct` in most examples, but the same approaches work with objects of any of the spectral classes from package 'photobiology'.

16.4.1 Task: plotting `source_spct` objects

We start with a very simple example, and later add layers to the plot little by little. We create a line plot, assign it to a variable called `fig_sun.e0` and then on the next line `print` it[2]. We obtain a plot with the axis labeled with the names of the variables, which is enough to check the data, but not good enough for publication.

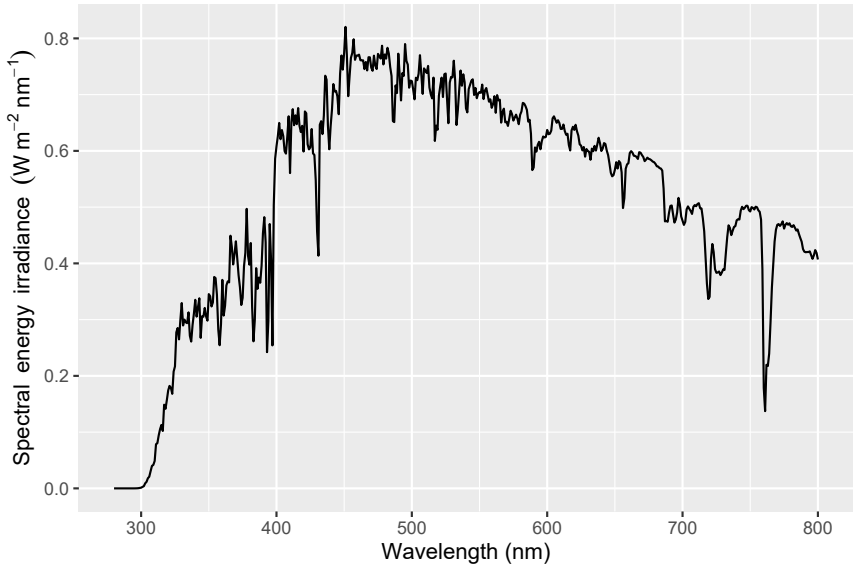
```
fig_sun.e0 <-
  ggplot(data=sun.spct, aes(x=w.length, y=s.e.irrad)) +
  geom_line()
fig_sun.e0
```

[2]we could have used `print(fig_sun.e0)` explicitly, but this is needed only in scripts because printing takes places automatically when working at the R console.



Next we add `labs` to obtain nicer axis labels, instead of assigning the result to a variable for reuse, we print it on-the-fly. As we need superscripts for the y-label we have to use `expression` instead of a character string as we use for the x-label. The syntax of expressions is complex, so please look at the documentation with `help(plotmath)` or read a book or watch tutorial for more details.

```
fig_sun.e0  +
  labs(
    y = expression(Spectral~~energy~~irradiance~~(W~m^{-2}~nm^{-1})),
    x = "Wavelength (nm)")
```



16.4.2 Task: Saving axis-label definitions for re-use

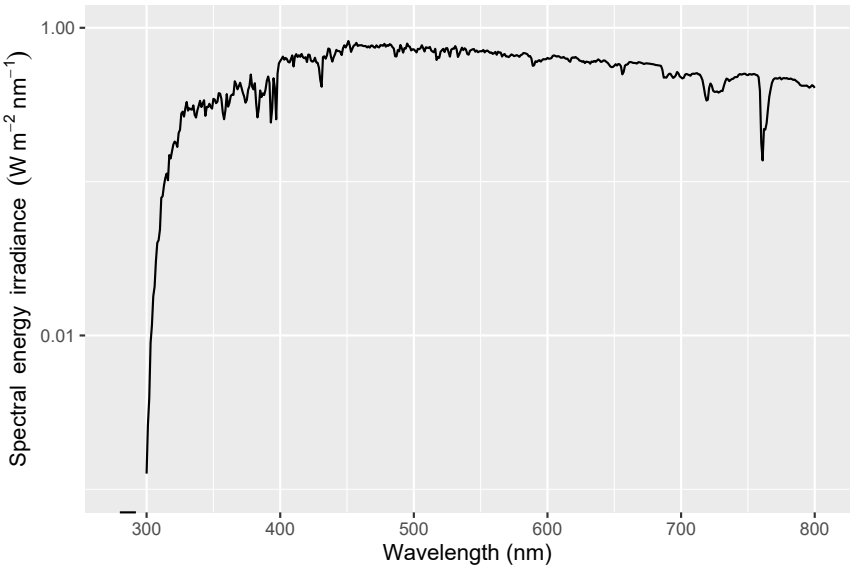
As we are going to re-use the same axis-labels in later plots, it is handy to save their definitions to variables. These definitions will be used in many of this chapter's plots. We also add `atop` to two of the expressions to obtain shorter versions by setting the spectral irradiance units on a second line in the axis labels.

```
ylab_watt <-
  expression(Spectral~~energy~~irradiance~~(W~m^{-2}~nm^{-1}))
ylab_watt_atop <-
  expression(atop(Spectral~~energy~~irradiance,
                  (W~m^{-2}~nm^{-1})))
ylab_umol <-
  expression(Spectral~~photon~~irradiance~~(mu*mol~m^{-2}~s^{-1}~nm^{-1}))
ylab_umol_atop <-
  expression(atop(Spectral~~photon~~irradiance,
                  (mu*mol~m^{-2}~s^{-1}~nm^{-1})))
xlab_nm <- "Wavelength (nm)"
```

16.4.3 Task: using a log scale

Here without need to recreate the figure, we add a logarithmic scale for the y-axis and print on the fly the result, and two of the just saved axis-labels. In this case we override the automatic limits of the scale. We do not give further examples of this, but could be also used with later examples, just by adjusting the values used as scale limits.

```
fig_sun.e0 +
  scale_y_log10(limits=c(1e-3, 1e0)) +
  labs(x = xlab_nm, y = ylab_watt)
```



The code above generates some harmless warnings, which are due some y values not being valid input for `log10`, the function used for the re-scaling, or because they fall outside the scale limits.

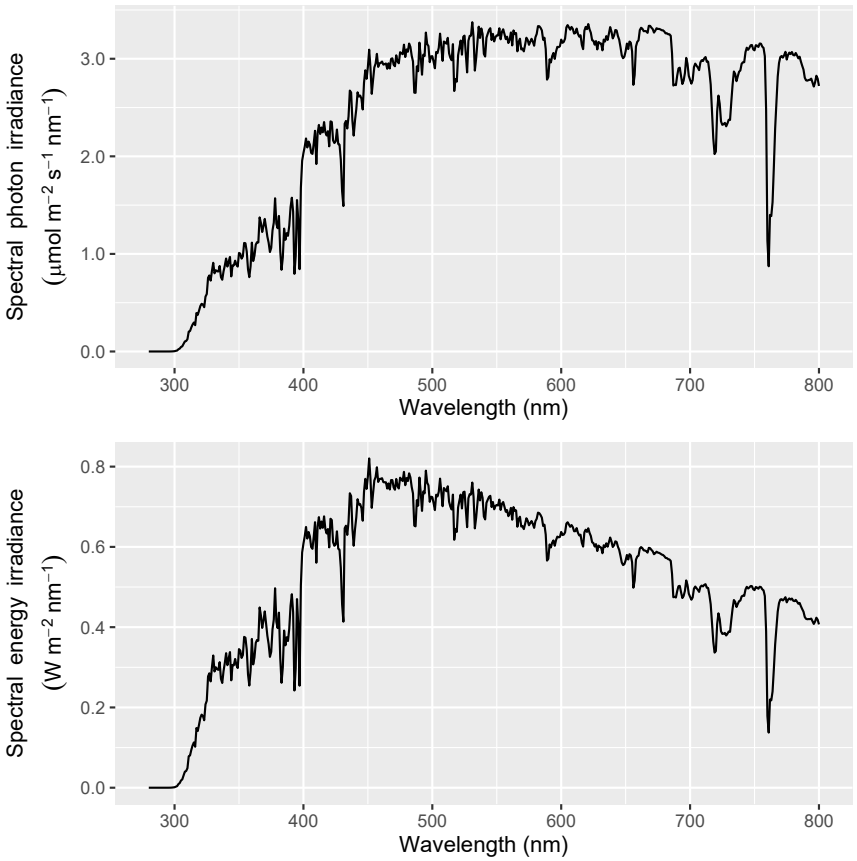
16.4.4 Task: compare energy and photon spectral units

We use once more the axis-labels saved above, but this time use the two-line label for the y-axis. To make sure that the width of the plotting area of both plots is the same, we need to have tick labels of the same width and format in both plots. For this we define a formatting function `num_one_dec` and then use it in the scale definition.

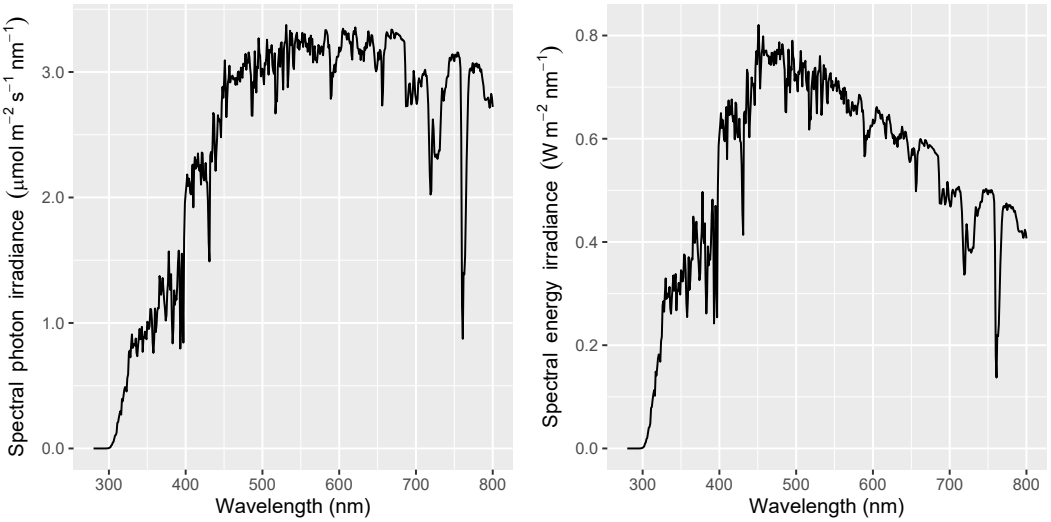
```
num_one_dec <- function(x, ...) {
  format(x, nsmall=1, trim=FALSE, width=4, ...)
  }

fig_sun.q <-
  ggplot(data=sun.spct, aes(x=w.length, y=s.q.irrad * 1e6)) +
  geom_line() +
  scale_y_continuous(labels = num_one_dec) +
  labs(x = xlab_nm)

fig_sun.e1 <-
  ggplot(data=sun.spct, aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  scale_y_continuous(labels = num_one_dec) +
  labs(x = xlab_nm)
```

We can use function `multiplot` to make a single plot from two separate ggplot objects, and put them side by or on top of each other. We use different y-axis labels in the two cases to make better use of the available space.

```
multiplot(fig_sun.q  + labs(y = ylab_umol_atop),
          fig_sun.e1 + labs(y = ylab_watt_atop),
          cols = 1)
```




```
multiplot(fig_sun.q  + labs(y = ylab_umol),
          fig_sun.e1 + labs(y = ylab_watt),
          cols = 2)
```

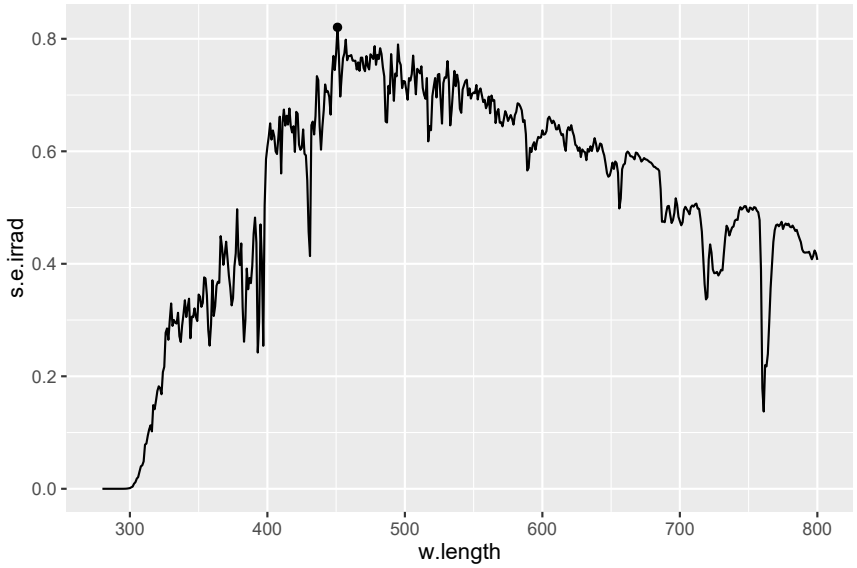


16.4.5 Task: annotating peaks and valleys in spectra

Here we show an example of the use of `stat_peaks` and `stat_valleys` from package 'ggspectra'. It uses the same parameter names and take the same arguments as methods `peaks` and `valleys` described in section **??**—please, consult this section for details on how to adjust how many and which local maxima and local minima are highlighted.

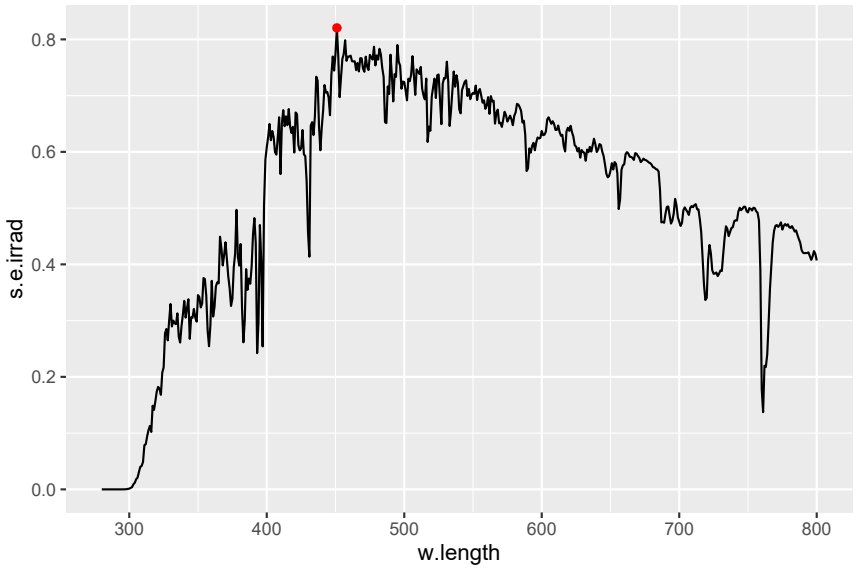
We reuse once more `fig_sun.e` saved in section 16.4 and we start with the simple example of highlighting the overall maximum in a spectrum. By default `geom_point` is used.

```
fig_sun.e0 + stat_peaks(span=NULL)
```



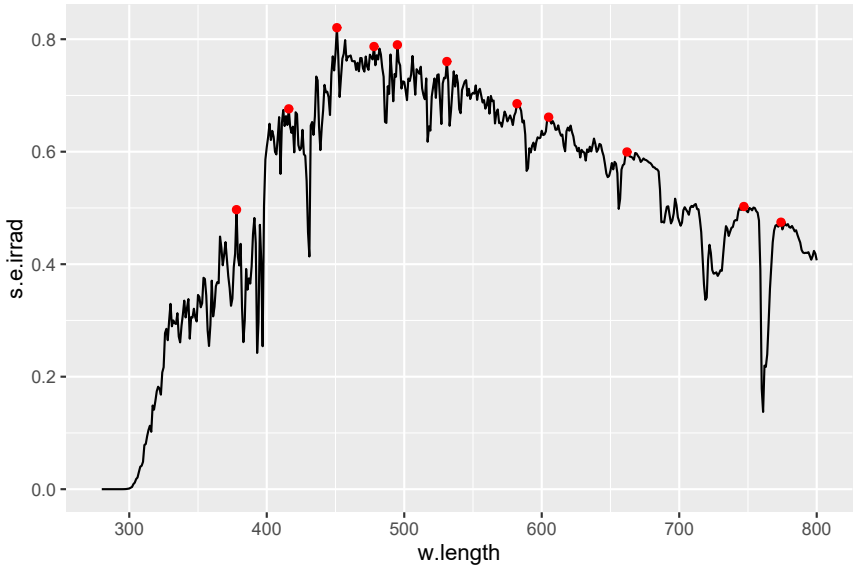
We can change aesthetics, for example the colour.

```
fig_sun.e0 + stat_peaks(span=NULL, color = "red")
```



The span, is the number of consecutive wavelength values in the data used to locate each individual maximum. The larger the value used, the 'coarser' the features detected. It is frequently needed to override the default so as to have only the "meaningful" features highlighted.

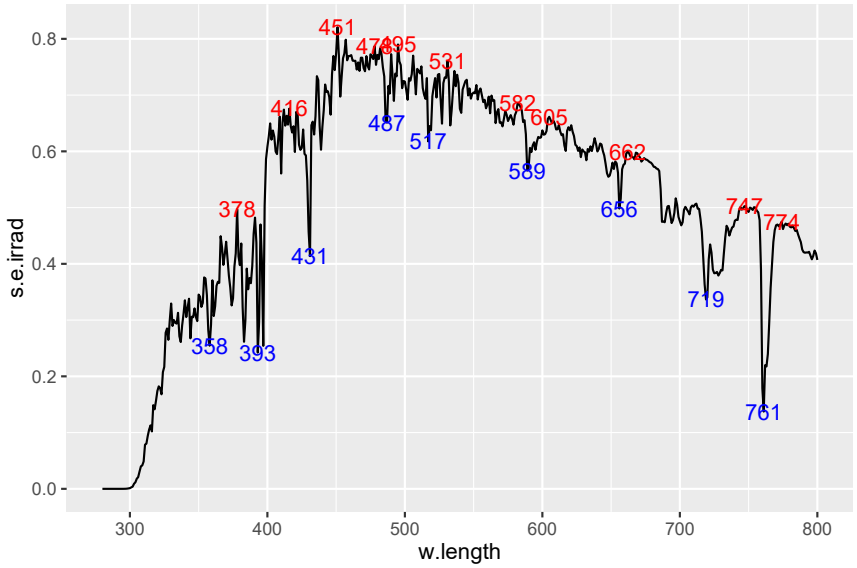
```
fig_sun.e0 + stat_peaks(span=31, color = "red")
```



Below we continue 'playing' with package 'ggplot2' to show different ways of plotting the peaks and valleys. Being a 'ggplot2'-compatible `stat_peaks` and `stat_valleys` accept a `geom` argument and all the aesthetics valid for the chosen `geom`. By overriding the default geom argument `"point"` with `"text"` we obtain labels for peaks and valleys. Be aware that consistently with package 'ggplot2', the

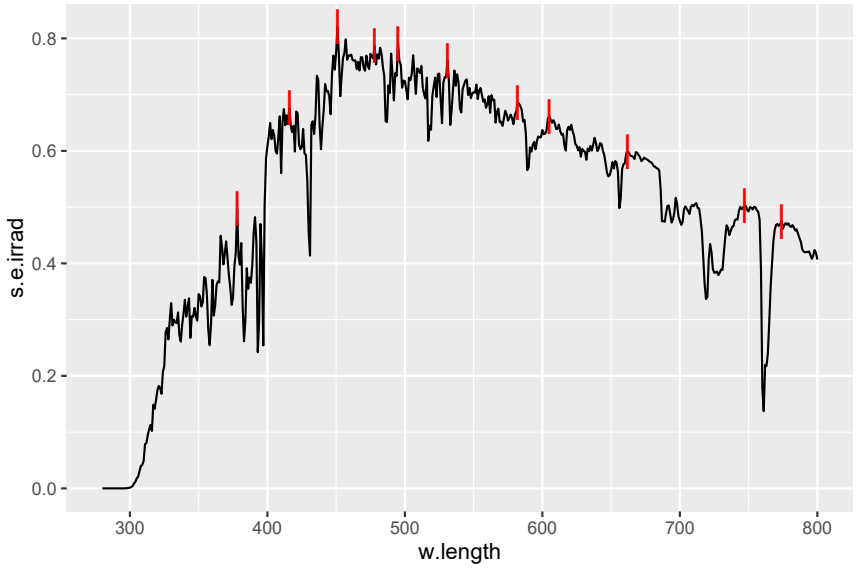
`geom` parameter takes as argument a character string giving the name of the `geom`, rather than the name of the function—in this case `geom_text`.

```
fig_sun.e0 + stat_peaks(geom = "text", colour="red", span=31) +
             stat_valleys(geom = "text", colour="blue", span=51)
```



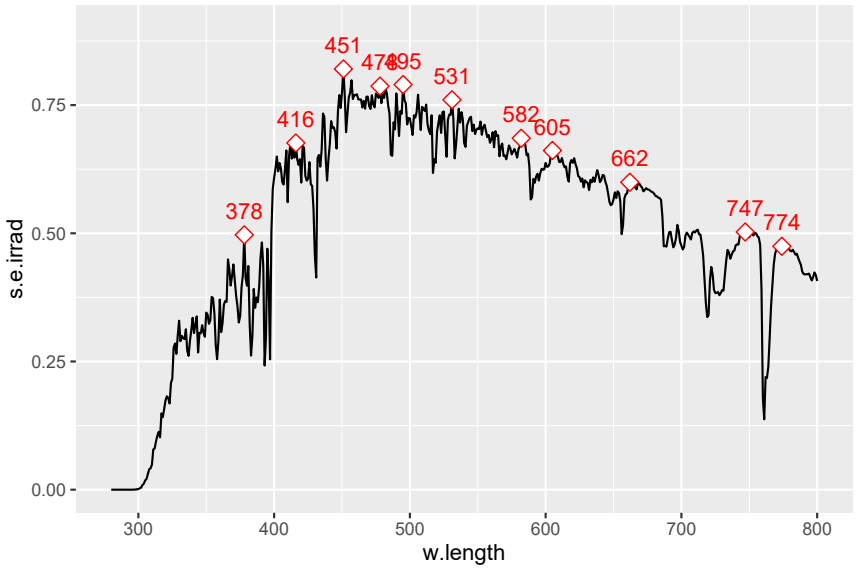
We can use the default `geom`, `geom_point`, change a few additional aesthetics: we set `shape` to a character, and set its size to 6.

```
fig_sun.e0 +
  stat_peaks(colour="red", geom="point",
             shape="|", size=6, span=31)
```



We can add the same `stat` two or more times to a `ggplot` object, in this example, each time with a different `geom`. First we add points to mark the peaks, and afterwards add labels showing the wavelengths at which they are located using geom `"text"`. For the `shape`, or type of symbol, we use one that supports 'fill', and set the `fill` to `"white"` but keep the border of the symbol `"red"` by setting `colour`, we also change the `size`. With the labels we use `vjust` to 'justify' the text moving the labels vertically, so that they do not overlap the line depicting the spectrum[3] In addition we expand the y-axis scale so that all labels fall within the plotting area.

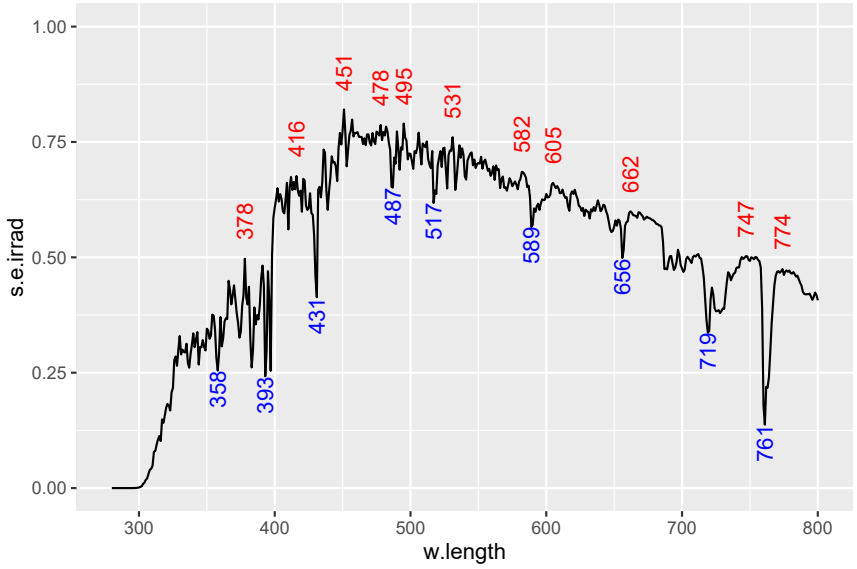
```
fig_sun.e0 +
  stat_peaks(colour="red", geom="point", shape=23,
             fill="white", size=3, span=31) +
  stat_peaks(colour="red", geom="text", vjust=-1, span=31) +
  expand_limits(y=0.9)
```



Finally an example with rotated labels, using different colours for peaks and valleys. Be aware that the 'justification' direction, as discussed in the footnote, is referenced to the position of the text, and for this reason to move the rotated labels upwards we need to use `hjust` as the desired displacement is horizontal with respect to the orientation of the text of the label. As we put peak labels above the spectrum and valleys bellow it, we need to use `hjust` values of opposite sign, but the exact values used were simply adjusted by trial and error until the figure looked as desired.

[3]The default position of labels is to have them centred on the coordinates of the peak or valley. Unless we rotate the label, `vjust` can be used to shift the label along the y-axis, however, justification is a property of the text, not the plot, so the vertical direction is referenced to the position of the text of the label. A value of 0.5 indicates centering, a negative value 'up' and a positive value 'down'. For example a value of -1 puts the x, y coordinates of the peak or valley at the lower edge of the 'bounding box' of the text. For `hjust` values of -1 and 1 right and left justify the label with respect to the x, y coordinates supplied. Values other than -1, 0.5, and 1, are valid input, but are rather tricky to use for `hjust` as the displacement is computed relative to the width of the bounding box of the label, the displacement being different for the same numerical value depending on the length of the label text.

```
fig_sun.e0 +
  stat_peaks(geom = "text", angle=90, hjust=-0.5, colour="red", span=31) +
  stat_valleys(geom = "text", angle=90, hjust=1, color="blue", span=51) +
  expand_limits(y=1.0)
```



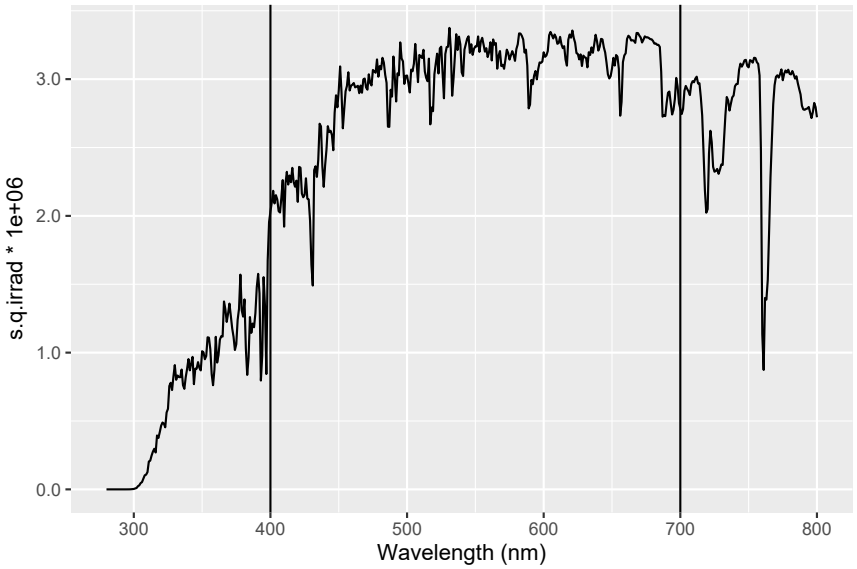
See section **??** in chapter 22 for an example these stats together with facets.

16.4.6 Task: annotating wavebands

THIS SECTION NEEDS TO BE RE-WRITTEN USING CURRENT VERSION OF 'ggspectra'.

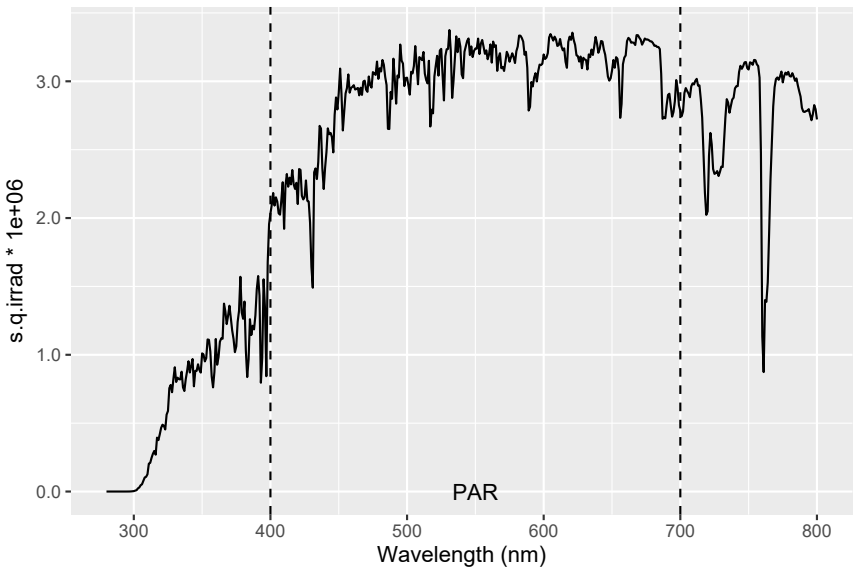
A simple example using `geom_vline` and method `range` with a `waveband` object as argument.

```
figvl3 <- fig_sun.q +
  geom_vline(xintercept=range(PAR()))

figvl3
```



And one where we change some of the aesthetics in the previous figure, and add a label using `stat_wb_label` defined in package 'ggspectra'.

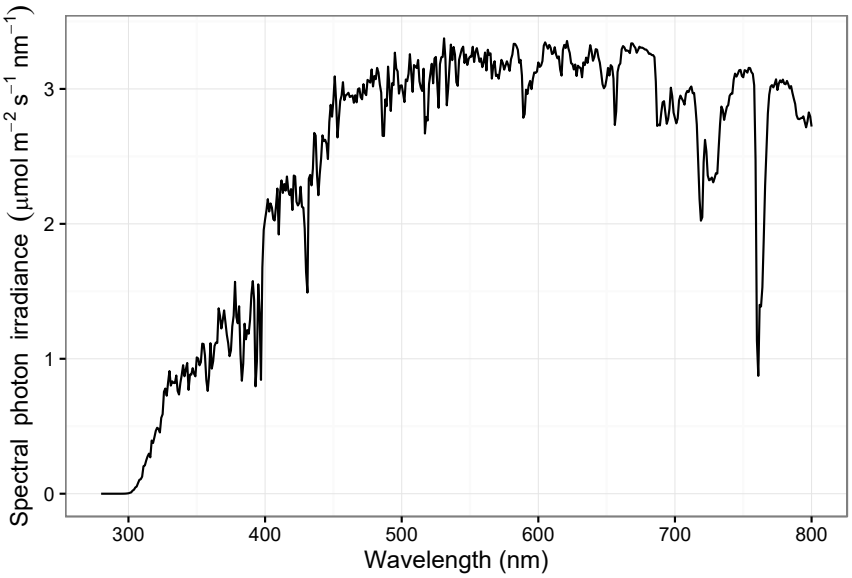
```
figvl4 <- fig_sun.q +
  geom_vline(xintercept=range(PAR()), linetype="dashed") +
  stat_wb_label(w.band = PAR())

figvl4
```



Next we use calculated values in the label, first with a simple example with only PAR. Because we use expressions to obtain superscripts we need to add `parse=TRUE` to the call. In addition as we are expressing the integral in photon based units, we also change the type of units used for plotting the spectral irradiance (multiplying by

$1 \cdot 10^6$ to because of the unit multiplier used).

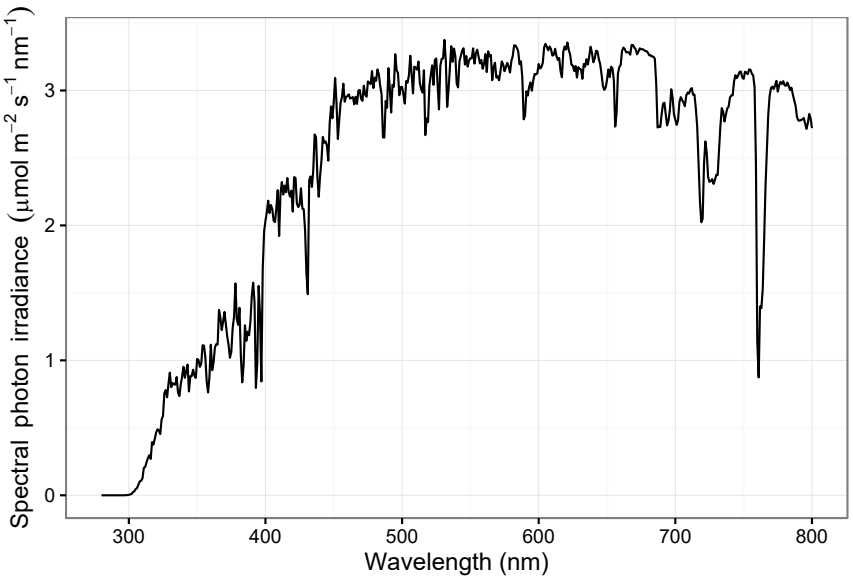
```
fig_sun <- ggplot(data=sun.spct,
                  aes(x=w.length, y=s.q.irrad * 1e6)) +
  geom_line() +
  labs(y = ylab_umol,
       x = "Wavelength (nm)")

# par <- q_irrad(sun.spct, PAR()) * 1e6
#
 fig_sun2 <- fig_sun # +
#   annotate_waveband(PAR(), "rect", ymax=3.5) +
#   annotate_waveband(PAR(), "text",
#                     label=paste("PAR:~", signif(par,digits=2),
#                                 "*~mu*mol~m^{-2}~s^{-1}", sep=""),
#                     y=3.75, colour="black", parse=TRUE)

fig_sun2 + theme_bw()
```



A variation of the previous figure shows how to use smaller rectangles for annotation, which yields plots where the spectrum itself is easier to see than when the rectangle overlaps the spectrum. We achieve this by supplying as argument both `ymax` and `ymin`, and slightly reducing the size of the text with `size = 4`.

```
fig_sun <- ggplot(data=sun.spct,
                  aes(x=w.length, y=s.q.irrad * 1e6)) +
  geom_line() +
  labs(y = ylab_umol,
       x = "Wavelength (nm)")

par <- q_irrad(sun.spct, PAR()) * 1e6

fig_sun2 <- fig_sun # +
#   annotate_waveband(PAR(), "rect", ymax=3.95, ymin=3.55) +
#   annotate_waveband(PAR(), "text", size=4,
#                     label=paste("PAR:~", signif(par,digits=2),
```

```
#                                   "*~mu*mol~m^{-2}~s^{-1}", sep=""),
#                       y=3.75, colour="black", parse=TRUE)

fig_sun2 + theme_bw()
```



This type of annotations can be also easily done for effective exposures or doses, but in this example as we position the annotations manually, we can use ggplot2's 'normal' `annotate` function. We use `xlim` to restrict the plotted region of the spectrum to the range of wavelengths of interest.

```
fig_dsun <-
  ggplot(data=sun.daily.spct * yellow_gel.spct,
         aes(x=w.length, y=s.e.irrad * 1e-3)) + geom_line() +
  geom_line(data=sun.daily.spct * polyester.spct,
            colour="red") +
  labs(y =
   expression(Spectral~~energy~~exposure~~(kJ~m^{-2}~d^{-1}~nm^{-1})),
       x = "Wavelength (nm)") + xlim(290, 425) + ylim(0, 25)

cie.pe <-
  e_irrad(sun.daily.spct * polythene.spct, CIE()) * 1e-3
cie.ps <-
  e_irrad(sun.daily.spct * polyester.spct, CIE()) * 1e-3
cie.pc <-
  e_irrad(sun.daily.spct * PC.spct, CIE()) * 1e-3
y.pos <- 22.5

fig_dsun2 <- fig_dsun +
  annotate("text",
           label=paste("Polythene~~filter~~CIE:~",
                       signif(cie.pe, digits=3),
                       "*~kJ~m^{-2}~d^{-1}", sep=""),
           y=y.pos+2, x=300, hjust=0, colour="black",
           parse=TRUE) +
  annotate("text", label=paste("Polyester~~filter~~CIE:~",
                               signif(cie.ps, digits=3),
```

```
                              "*~kJ~m^{-2}~d^{-1}", sep=""),
           y=y.pos, x=300,  hjust=0,  colour="red",
           parse=TRUE) +
  annotate("text", label=paste("Polycarbonate~~filter~~CIE:~",
                               signif(cie.pc, digits=3),
                               "*~kJ~m^{-2}~d^{-1}", sep=""),
           y=y.pos-2, x=300, hjust=0,  colour="blue",
           parse=TRUE)

fig_dsun2 + theme_bw()
```

16.5 Using colour as data in plots

The examples in this section use a single spectrum, `sun.spct`, but all functions used are methods for `generiic.spct` objects, so are equally applicable to the plotting of other spectra like transmittance, reflectance or response ones.

When we want to colour-label individual spectral values, for example, by plotting the individual data points with the colour corresponding to their wavelengths, or fill the area below a plotted spectral curve with colours, we need to first `tag` the spectral data set using a waveband definition or a list of waveband definitions. If we just want to add a guide or labels to the plot, we can create new data instead of tagging the spectral data to be plotted. In section 16.5.1 we show code based on tagging spectral data, and in section 16.5.2 the case of using different data for plotting the guide or key is described.

16.5.1 Task: Plots using colour for the spectral data

We start by describing how to tag a spectrum, and then show how to use tagged spectra for plotting data. Tagging consist in adding wavelength-derived colour data and waveband-related data to a spectral object. We start with a very simple example.

```
cp.sun.spct <- tag(sun.spct)
```

As no waveband information was supplied as input, only wavelength-dependent colour information is added to the spectrum plus a factor `wb.f` with only `NA` level.

If we instead provide a waveband as input then both wavelength-dependent colour and waveband information are added to the spectral data object.

```
uvb.sun.spct <- tag(sun.spct, UVB())
levels(uvb.sun.spct[["wb.f"]])

## [1] "UVB"
```

The output contains the same variables (columns) but now the factor `wb.f` has a level based on the name of the waveband, and a value of `NA` outside it.

We can alter the name used for the `wb.f` factor levels by using a named list as argument.

```
uvb.sun.spct <- tag(uvb.sun.spct, list('ultraviolet-B' = UVB()))

##  Warning  in  tag.generic_spct(uvb.sun.spct,  list(`ultraviolet-B`  =  UVB())):
Overwriting old tags in spectrum

levels(uvb.sun.spct[["wb.f"]])

## [1] "UVB"
```

This example also shows, that re-tagging a spectrum replaces the old tagging data with the new one.

If we use a list of wavebands then the tagging is based on all of them, but be aware that the wavelength ranges of the wavebands overlap, the result is undefined.

```
plant.sun.spct <- tag(sun.spct, Plant_bands())
levels(plant.sun.spct[["wb.f"]])

## [1] "UVB"   "UVA"   "Blue"  "Green" "R"
## [6] "FR"
```

Tagging also adds some additional data as an attribute to the spectrum. This data can be retrieved with the base R function `attr`.

```
attr(cp.sun.spct, "spct.tag")

## $time.unit
## [1] "second"
##
## $wb.key.name
## [1] "Bands"
##
## $wl.color
## [1] TRUE
##
## $wb.color
## [1] TRUE
##
## $wb.num
## [1] 1
##
## $wb.colors
## [1] "#554340"
##
## $wb.names
## [1] "Total"
##
## $wb.list
## $wb.list[[1]]
## Total
## low (nm) 280
## high (nm) 800
## weighted none

attr(uvb.sun.spct, "spct.tag")

## $time.unit
## [1] "second"
##
```

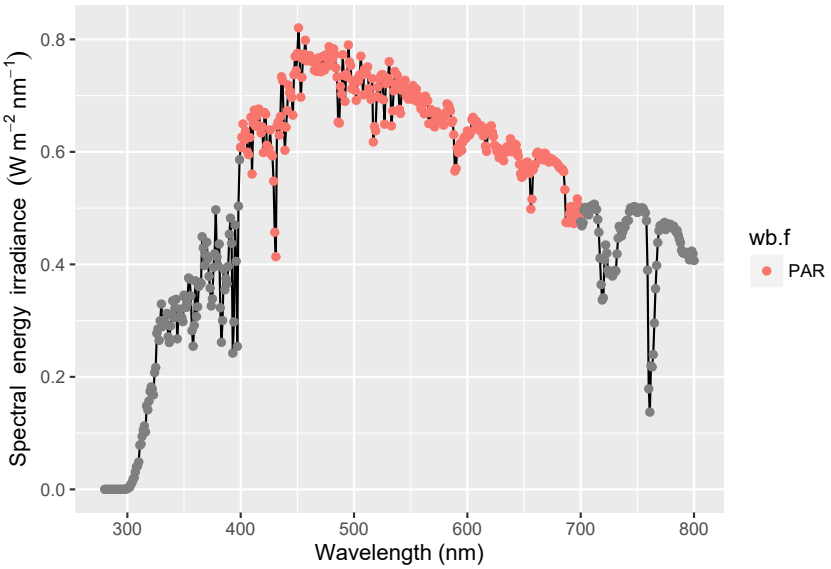
```
## $wb.key.name
## [1] "Bands"
##
## $wl.color
## [1] TRUE
##
## $wb.color
## [1] TRUE
##
## $wb.num
## [1] 1
##
## $wb.colors
## [1] "black"
##
## $wb.names
## [1] "UVB"
##
## $wb.list
## $wb.list[[1]]
## UVB.ISO
## low (nm) 280
## high (nm) 315
## weighted none
```

We now tag a spectrum for use in our first plot example.

```
par.sun.spct <- tag(sun.spct, PAR())
```

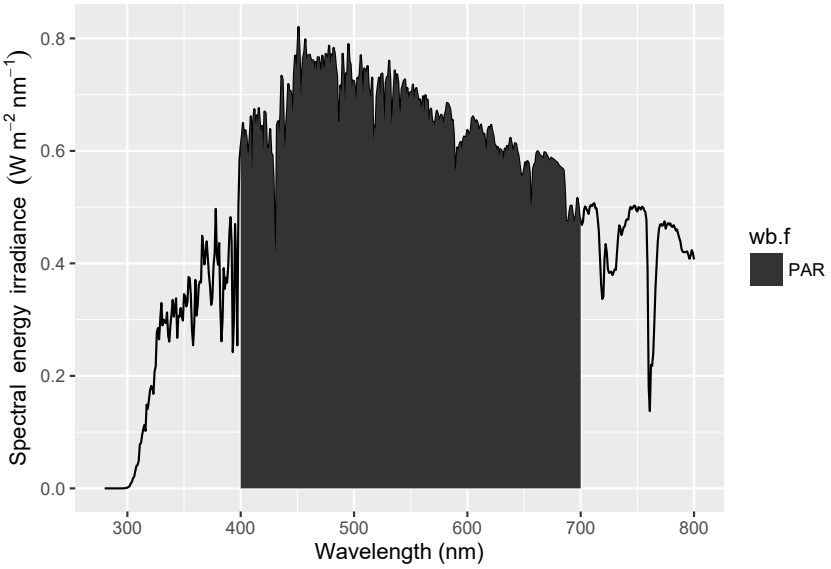
Here we simply use the `wb.f` factor that was added as part of the tagging, with the default colour scale of 'ggplot2', which results in a palette unrelated to the real colour of the different wavelengths.

```
fig_sun.t00 <-
  ggplot(data=par.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  geom_point(aes(color=wb.f)) +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.t00
```



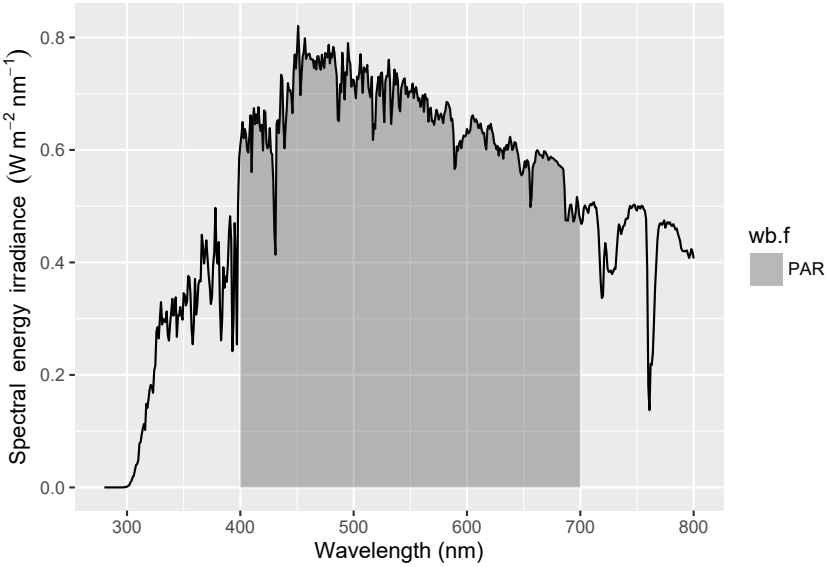
We can also use other `geom`s like `geom_area` in the next chunk, together with, as an example, a grey fill scale from 'ggplot2'.

```
fig_sun.t01 <-
  ggplot(data=par.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  geom_area(color=NA, aes(fill=wb.f)) +
  scale_fill_grey(na.value=NA) +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.t01
```



The default fill looks too dark and bold, so we change the transparency of the fill by setting `fill = 0.3`. The grid in the background becomes slightly visible also in the filled region, facilitating 'reading' of the plot and avoiding a to stark contrast between regions, which tends to be disturbing. In later plots we frequently use `alpha` to improve how plots look, but we exemplify the effect of changing this aesthetic only here.

```
fig_sun.t01 <-
  ggplot(data=par.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  geom_area(color=NA, alpha=0.3, aes(fill=wb.f)) +
  scale_fill_grey(na.value=NA) +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.t01
```



As part of the tagging colour information was also added to the spectral data object[4]. We tag each observation in the solar spectrum with human vision colours as defined by ISO.

```
tg.sun.spct <- tag(sun.spct, VIS_bands())
```

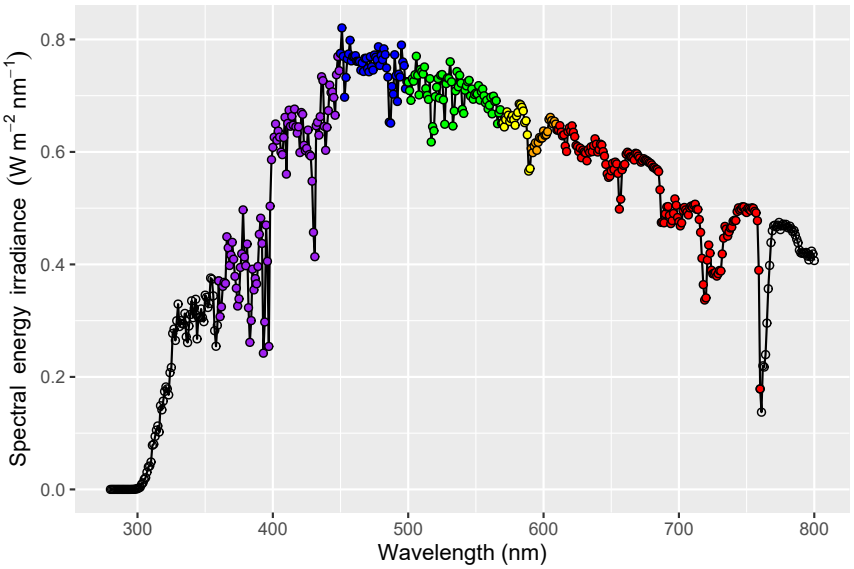
See section ?? on page ?? for the definition of the colour and fill scales used for tagged spectra. These definitions are needed for most of the plots in the remaining of the present and next sections. These scales retrieve information about the wavebands both from the data itself and from the attribute described above.

Here we plot using colours by waveband—using the colour definitions by ISO—, with symbols filled with colours. The colour data outside the wavebands is set to `NA`

[4]We may want to increase the number of 'observations' in the spectrum by interpolation if there are too few observations for a smooth colour gradient.

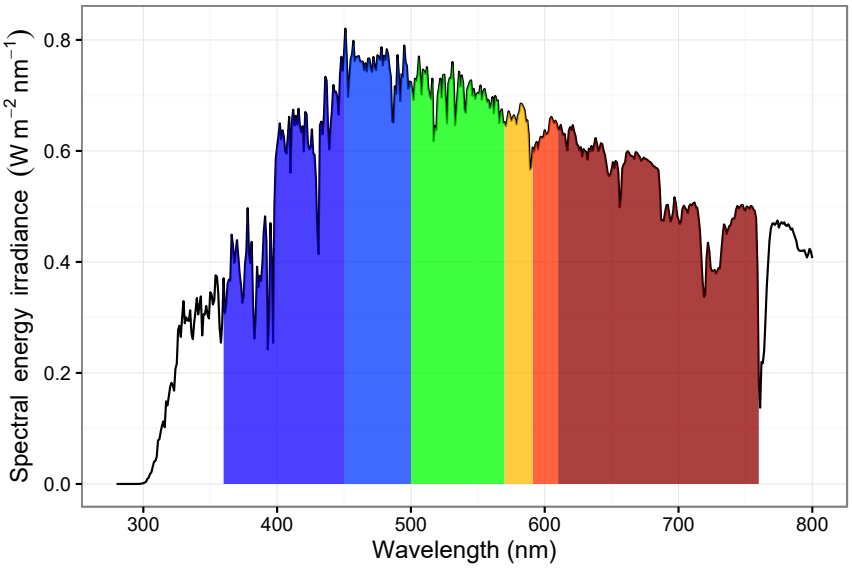
so those points are not filled. One can play with the `size` of points until ones get the result wanted. The default `shape`s used by 'ggplot2' do not accept a `fill` aesthetic, while shape '21' gives circles that can be 'filled'.

```
fig_sun.t02 <-
  ggplot(data=tg.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  scale_fill_identity() +
  geom_point(aes(fill=wb.f), shape=21)  +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.t02
```



Using `geom_area` we can fill the area under the curve according to the colour of different wavebands, we set the fill only for this geom, so that the `NA`s do not affect other plotting. To get a single black curve for the spectrum we use `geom_line`. This approach works as long as wavebands do not share the same value for the color, which means that it is not suitable either when more than one band is outside the visible range, or when using many narrow wavebands.

```
fig_sun.t03 <-
  ggplot(tg.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_fill_identity() +
  geom_line() +
  geom_area(aes(fill=wb.color), alpha=0.75) +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.t03 + theme_bw()
```

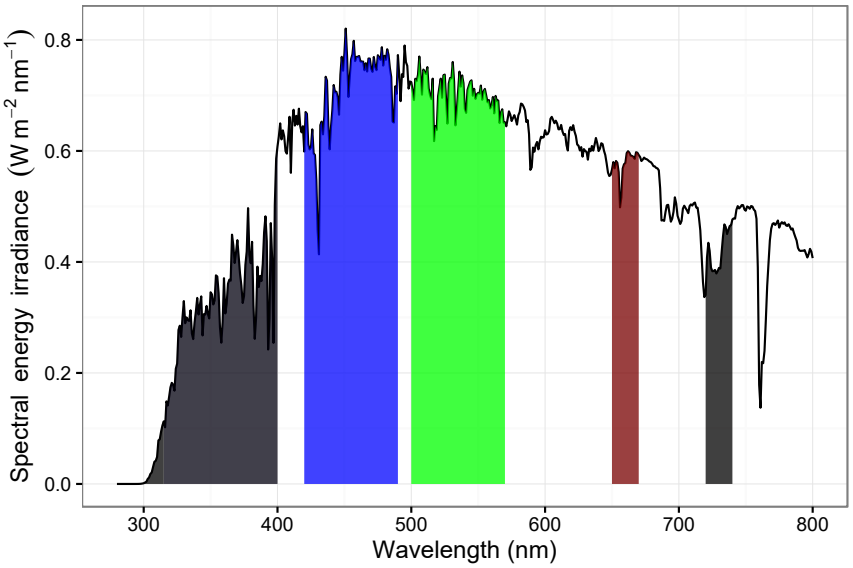


In the next example we tag the solar spectrum with colours using the definitions of plant sensory 'colours'.


```
pl.sun.spct <- tag(sun.spct, Plant_bands())
```

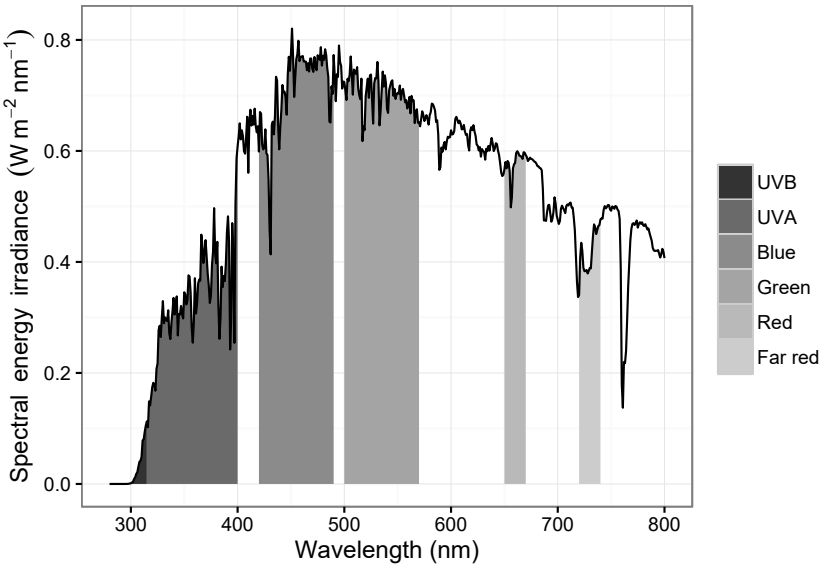
Here we plot the wavebands corresponding to plant sensory 'colours', using the spectrum we tagged in the previous code chunk.

```
fig_sun.pl0 <-
  ggplot(pl.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_fill_identity() +
  geom_line() +
  geom_area(aes(fill=wb.color), alpha=0.75) +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.pl0 + theme_bw()
```



We can also use the factor `wb.f` which has value `NA` outside the wavebands, changing the colour used for `NA` to `NA` which renders it invisible. We can change the labels used for the wavebands in two different way, when plotting by supplying a labels argument to the scale used, or when tagging the spectrum. The second approach is simpler when producing several different plots from the same spectral object, or when wanting to have consistent labels and names used also in derived results such as irradiance.

```
fig_sun.pl1 <-
  ggplot(pl.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_area(aes(fill=wb.f)) +
  scale_fill_grey(na.value=NA, name="",
                  labels=c("UVB", "UVA", "Blue",
                           "Green", "Red", "Far red")) +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.pl1 + theme_bw()
```



When using a factor we can play with the scale definitions and represent the wavebands in any way we may want. For example we can use `split_bands` to split a waveband or spectrum into many adjacent narrow bands and get an almost continuous gradient, but we need to get around the problem of repeated colours by using the factor and redefining the scale.

When an spectrum has very few observations we can 'fake' a longer spectrum by interpolation as a way of getting a more even fill. The example below is not run, in later examples we just use the example spectral data as is.

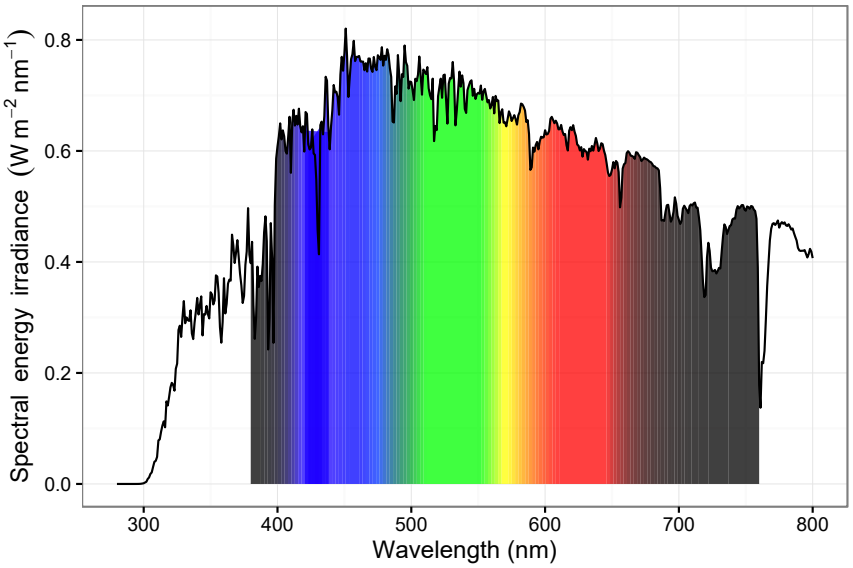
```
interpolate_spct(sun.spct, length.out=800)
```

We tag the VIS region of the spectrum with 150 narrow wavebands. As 'hinges' are inserted, there is no gap, and usually there is no need to increase the length of the spectrum by interpolation. If needed one could try something like. However, the longer spectrum should not be used for statistical calculations, not even plotting using `geom_smooth`.

```
splt.sun.spct <- tag(sun.spct, split_bands(VIS(), length.out=150))
```

In the code above, we made a copy of `sun.spct` using a different name so as not hide the object in package 'photobiology'.

```
fig_sun.splt0 <-
  ggplot(splt.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_fill_identity() +
  geom_area(aes(fill=wb.color), alpha=0.75) +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.splt0 + theme_bw()
```

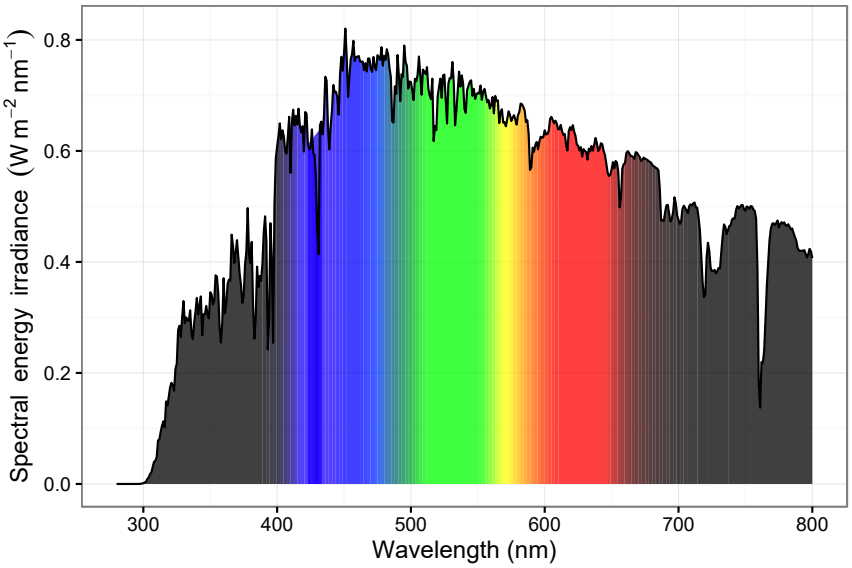


In this other example we tag the whole spectrum, dividing it into 200 wavebands.

```
splt1.sun.spct <- tag(sun.spct, split_bands(sun.spct, length.out=200))
```

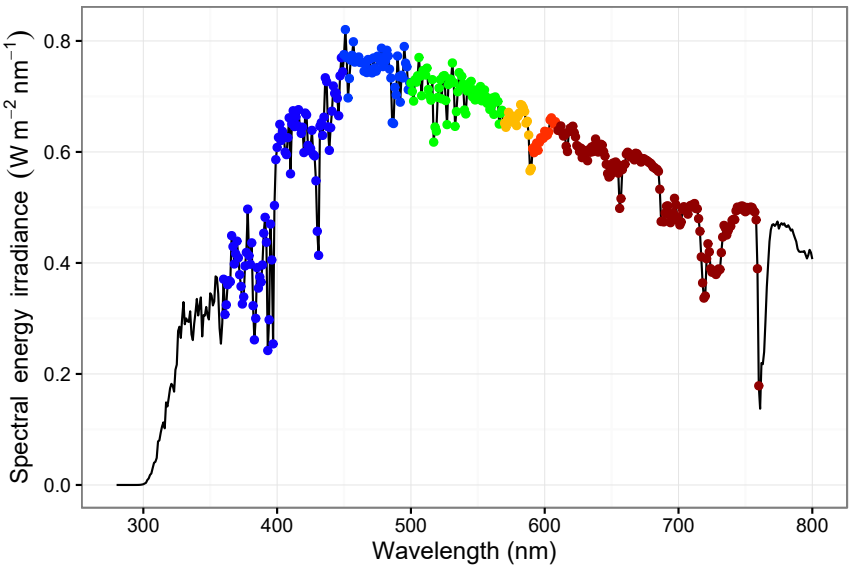
We use `geom_area` and `fill`, and colour the area under the curve. This does not work with `geom_line` because there would not be anything to fill, here we use `geom_area` instead.

```
fig_sun.splt1 <-
  ggplot(splt1.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_fill_identity() +
  geom_area(aes(fill=wb.color), alpha=0.75) +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.splt1 + theme_bw()
```



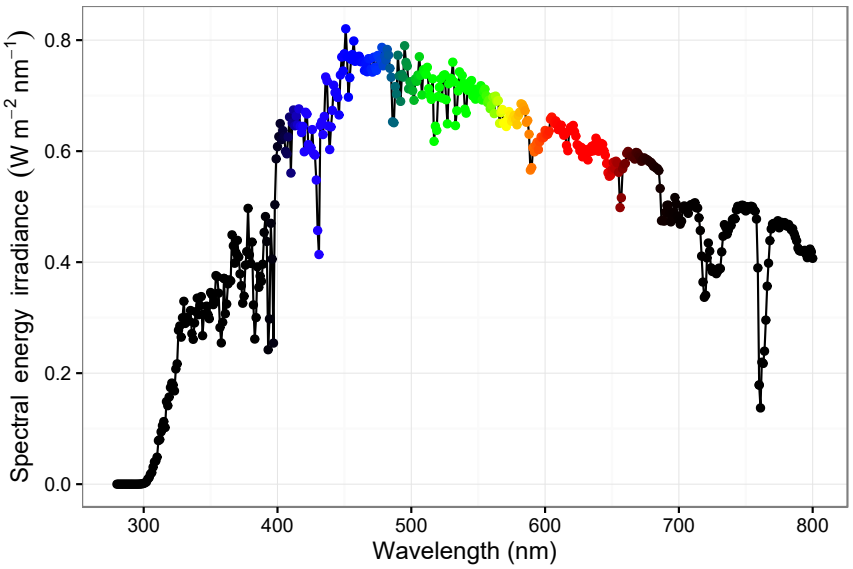
The next example uses `geom_point` and `colour` to color the data points according the waveband they are included in.

```
fig_sun.tg1 <-
  ggplot(tg.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_colour_identity() +
  geom_line() +
  geom_point(aes(colour=wb.color)) +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.tg1 + theme_bw()
```



When plotting points, rather than an area we may, instead of using colours from wavebands, want to plot the colour calculated for each individual wavelength value, which `tag` adds to the spectrum, whether a waveband definition is supplied or not. In this case we need to use `scale_color_identity`.

```
fig_sun.tg2 <-
  ggplot(data=tg.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  scale_color_identity() +
  geom_point(aes(color=wl.color))  +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.tg2  + theme_bw()
```



Other possibilities are for example, using one of the symbols that can be filled, and then for example for symbols with a black border and a colour matching its wavelength as a fill aesthetic. It is also possible to use `alpha` with points.

16.5.2 Task: Plots using waveband definitions

In the previous section we showed how tagging spectral data can be used to add colour information that can be used when plotting. In contrast, in the present section we create new 'fake' spectral data starting from waveband definitions that then we plot as 'annotations'. We show different types of annotations based on plotting with different `geom`s. We show the use of `geom_rect`, `geom_text`, `geom_vline`, and `geom_segment`, that we consider the most useful geometries in this context.

We use three different functions from package 'photobiology' to generate the data to be plotted from lists of waveband definitions. We use mainly pre-defined wavebands, but user defined wavebands can be used as well. We start by showing the

output of these functions, starting with `wb2spct` the simplest one.

```
wb2spct(PAR())

## Object: generic_spct [4 x 8]
## Wavelength range 400 to 700 nm, step 1.023182e-12 to 300 nm
##
## # A tibble: 4 x 8
##   w.length counts   cps s.e.irrad s.q.irrad   Tfr
##      <dbl>  <dbl> <dbl>     <dbl>     <dbl> <dbl>
## 1      400      0     0         0         0     0
## 2      400      0     0         0         0     0
## 3      700      0     0         0         0     0
## 4      700      0     0         0         0     0
## # ... with 2 more variables: Rfl <dbl>,
## #   s.e.response <dbl>

wb2spct(Plant_bands())

## Object: generic_spct [22 x 8]
## Wavelength range 280 to 740 nm, step 1.023182e-12 to 85 nm
##
## # A tibble: 22 x 8
##   w.length counts   cps s.e.irrad s.q.irrad   Tfr
##      <dbl>  <dbl> <dbl>     <dbl>     <dbl> <dbl>
## 1      280      0     0         0         0     0
## 2      280      0     0         0         0     0
## 3      315      0     0         0         0     0
## 4      315      0     0         0         0     0
## # ... with 18 more rows, and 2 more variables:
## #   Rfl <dbl>, s.e.response <dbl>
```

Function `wb2tagged_spct` returns the same 'spectrum', but tagged with the same wavebands as used to create the spectral data, and you will also notice that a 'hinge' has been added, which is redundant in the case of a single waveband, but needed in the case of wavebands sharing a limit.

```
wb2tagged_spct(PAR())

## Object: generic_spct [4 x 12]
## Wavelength range 400 to 700 nm, step 1.023182e-12 to 300 nm
##
## # A tibble: 4 x 12
##   w.length counts   cps s.e.irrad s.q.irrad   Tfr
##      <dbl>  <dbl> <dbl>     <dbl>     <dbl> <dbl>
## 1      400      0     0         0         0     0
## 2      400      0     0         0         0     0
## 3      700      0     0         0         0     0
## 4      700      0     0         0         0     0
## # ... with 6 more variables: Rfl <dbl>,
## #   s.e.response <dbl>, wl.color <chr>,
## #   wb.color <chr>, wb.f <fctr>, y <dbl>

wb2tagged_spct(Plant_bands())

## Object: generic_spct [22 x 12]
## Wavelength range 280 to 740 nm, step 1.023182e-12 to 85 nm
##
## # A tibble: 22 x 12
```

```
##   w.length counts   cps s.e.irrad s.q.irrad   Tfr
##      <dbl>  <dbl> <dbl>     <dbl>     <dbl> <dbl>
## 1      280      0     0         0         0     0
## 2      280      0     0         0         0     0
## 3      315      0     0         0         0     0
## 4      315      0     0         0         0     0
## # ... with 18 more rows, and 6 more variables:
## #   Rfl <dbl>, s.e.response <dbl>,
## #   wl.color <chr>, wb.color <chr>, wb.f <fctr>,
## #   y <dbl>
```

The third function, `wb2rect_spct` is what we use in most examples. It generates data that make it easier to plot rectangles with `geom_rect` as we will see in later examples.

```
wb2rect_spct(PAR())
```

```
## Object: generic_spct [1 x 15]
## Wavelength range 550 to 550 nm, step NA nm
##
## # A tibble: 1 x 15
##   w.length counts   cps s.e.irrad s.q.irrad   Tfr
##      <dbl>  <dbl> <dbl>     <dbl>     <dbl> <dbl>
## 1      550      0     0         0         0     0
## # ... with 9 more variables: Rfl <dbl>,
## #   s.e.response <dbl>, wl.color <chr>,
## #   wb.color <chr>, wb.name <chr>, wb.f <fctr>,
## #   wl.high <dbl>, wl.low <dbl>, y <dbl>
```

```
wb2rect_spct(Plant_bands())
```

```
## Object: generic_spct [6 x 15]
## Wavelength range 297.5 to 730 nm, step 60 to 125 nm
##
## # A tibble: 6 x 15
##   w.length counts   cps s.e.irrad s.q.irrad   Tfr
##      <dbl>  <dbl> <dbl>     <dbl>     <dbl> <dbl>
## 1    297.5      0     0         0         0     0
## 2    357.5      0     0         0         0     0
## 3    455.0      0     0         0         0     0
## 4    535.0      0     0         0         0     0
## # ... with 2 more rows, and 9 more variables:
## #   Rfl <dbl>, s.e.response <dbl>,
## #   wl.color <chr>, wb.color <chr>,
## #   wb.name <chr>, wb.f <fctr>, wl.high <dbl>,
## #   wl.low <dbl>, y <dbl>
```

In this case instead of two rows per waveband, we obtain only one row per waveband, with a `w.length` value corresponding to its midpoint but with two additional columns giving the low and high wavelength limits.

As we saw earlier for tagged spectra, additional data is stored in an attribute.

```
attr(wb2rect_spct(PAR()), "spct.tags")
```

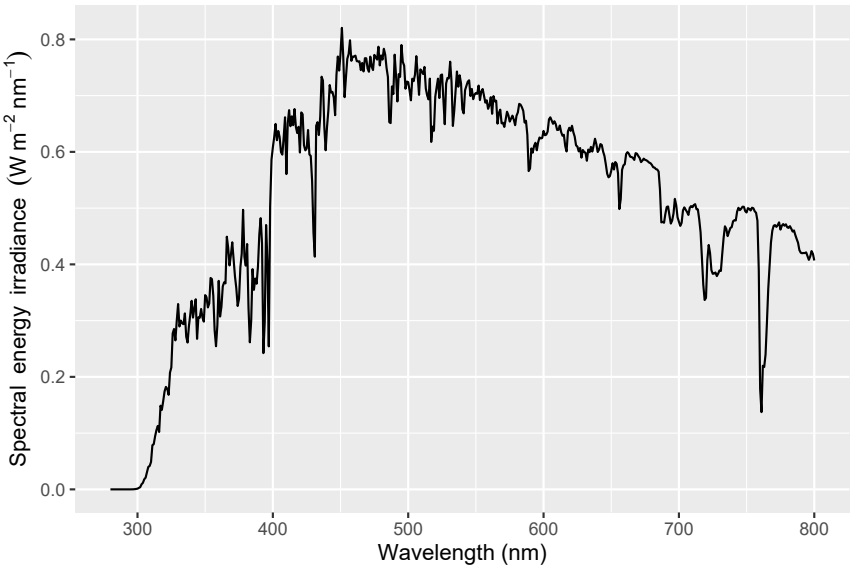
```
## $time.unit
## [1] "none"
##
```

```
## $wb.key.name
## [1] "Bands"
##
## $wl.color
## [1] TRUE
##
## $wb.color
## [1] TRUE
##
## $wb.num
## [1] 1
##
## $wb.colors
## [1] "#735B57"
##
## $wb.names
## [1] "PAR"
##
## $wb.list
## $wb.list[[1]]
## PAR
## low (nm) 400
## high (nm) 700
## weighted none
```


The first plot examples show how to add a colour bar as key. We create new data for use in what is closer to the concept of annotation that to plotting. In most of the examples below we use waveband definitions to create tagged spectral data for use in plotting the guide using `geom_rect`. We present three cases: an almost continuous colour reference guide, a reference guide for colours perceived by plants and one for ISO colour definitions. We also add labels to the bar with `geom_text` and show some examples of how to change the color of the line enclosing the rectangles and of text labels. Finally we show how to use `fill` and `alpha` to adjust how the guides look. Later on we show some examples using other `geom`s and also examples combining the use of tagged spectra as described in the previous section with the 'annotations' described here.

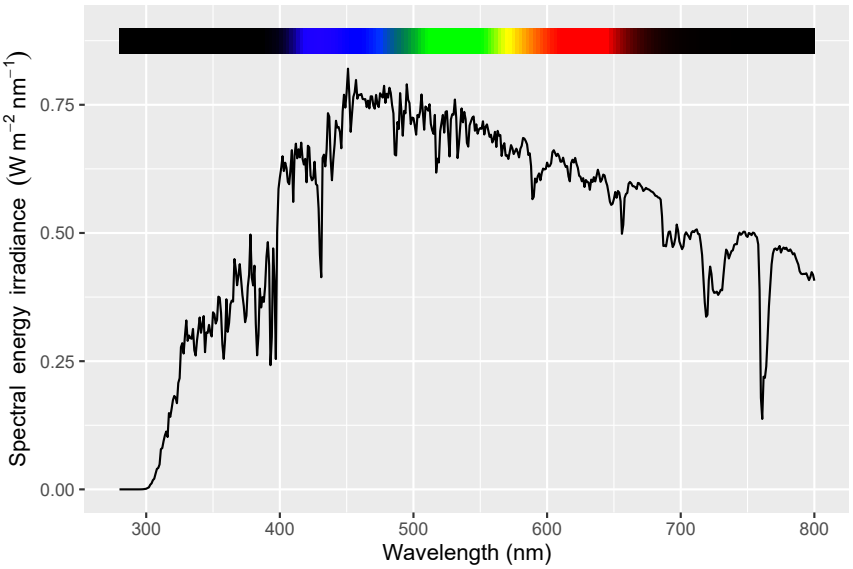
First we create a simple line plot of the solar spectrum, that we will use as a basis for most of the examples below.

```
fig_sun.z0 <-
  ggplot(data=sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.z0
```



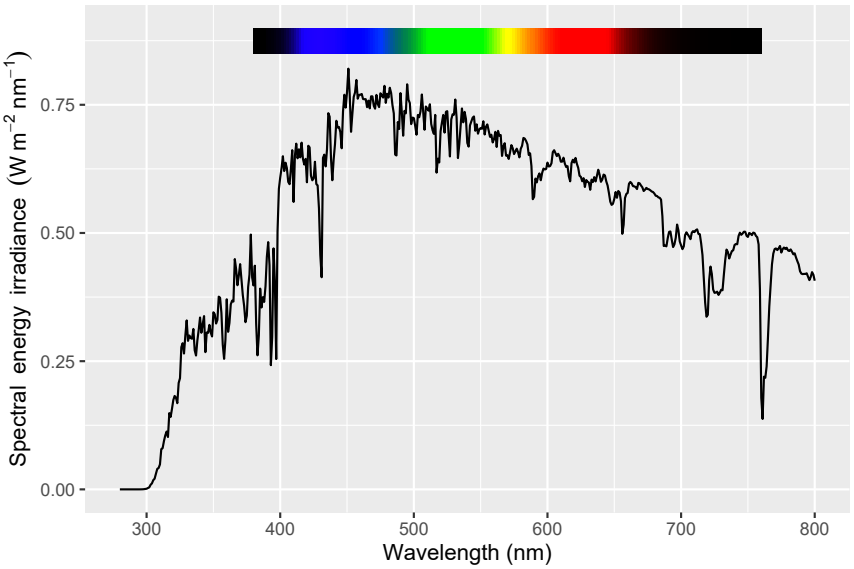
We now add to the plot created above a nearly continuous colour bar for the whole spectrum. To obtain an almost continuous colour scale we use a list of 200 wavebands. We need to specify `color = NA` to prevent the line enclosing each of the 200 rectangles from being plotted. We position the bar at the top because we think that it looks best, but by changing the values supplied to `ymax` and `ymin` move the bar vertically and also change its width.

```
wl.guide.spct <-
  wb2rect_spct(split_bands(sun.spct,
                           length.out=200))

fig_sun.z2 <- fig_sun.z0 +
  geom_rect(data=wl.guide.spct,
            aes(xmin = wl.low, xmax = wl.high,
                ymin = y + 0.85, ymax = y + 0.9,
                y = 0, fill=wb.color),
            color = NA) +
  scale_fill_identity()

fig_sun.z2
```



This second example differs very little from the previous one, but by using a waveband definition instead of a spectrum as argument to `split_bands`, we restrict the region covered by the colour fill to that of the waveband. In fax a vector of length two, or any object for which a `range` method is available can be used as input to this function.

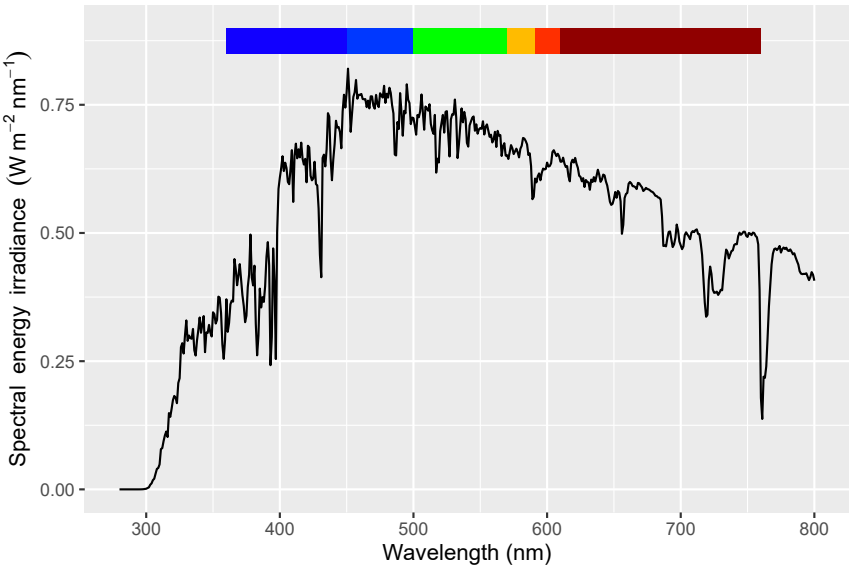
```
wl.guide.spct <- wb2rect_spct(split_bands(VIS(), length.out=200))

fig_sun.z1 <- fig_sun.z0 +
  geom_rect(data=wl.guide.spct,
            aes(xmin = wl.low, xmax = wl.high,
                ymin = y + 0.85, ymax = y + 0.9,
                y = 0, fill=wb.color),
            color = NA) +
  scale_fill_identity()

fig_sun.z1
```



In the examples above we have used a list of 200 waveband definitions created with `split_bands`. If we instead use a shorter list of definitions, we get a plot where the wavebands are clearly distinguished. By default if the list of wavebands is short, a key or 'guide' is also added to the plot.

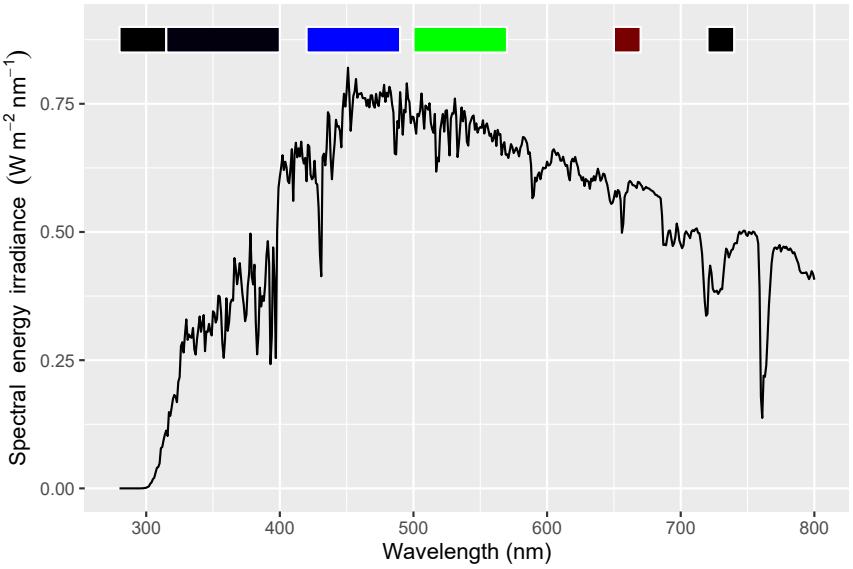
To demonstrate this we replace in the previous example, the previous tagged spectrum with one based on ISO colours. We need to do this replacement in the calls to both `geom_rect` and `scale_fill_tgspct`.

```
iso.guide.spct <- wb2rect_spct(VIS_bands())

fig_sun.z3 <- fig_sun.z0 +
  geom_rect(data=iso.guide.spct,
            aes(xmin = wl.low, xmax = wl.high,
                ymin = y + 0.85, ymax = y + 0.9,
                y = 0, fill=wb.color),
            color = NA) +
  scale_fill_identity()

fig_sun.z3
```



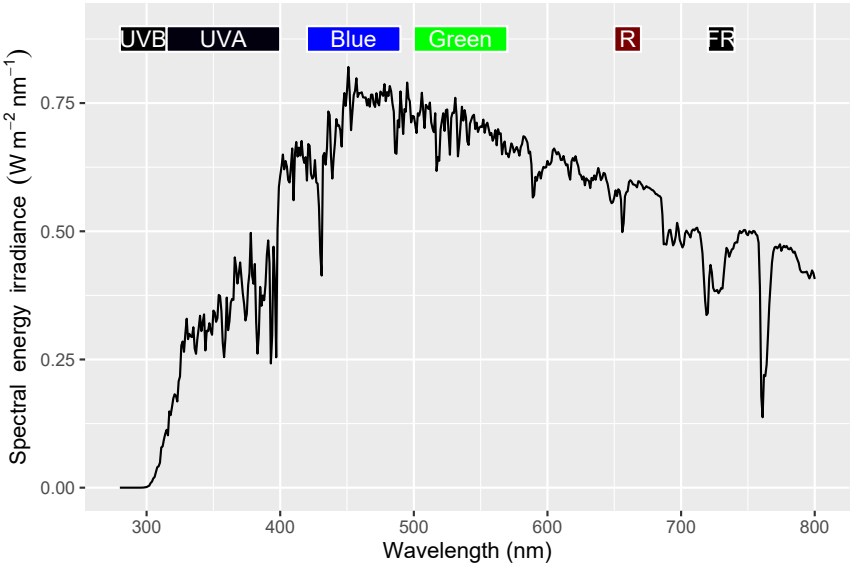
We use as an example plant's sensory colours, to show the case when the wavebands in the list are not contiguous.

```
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z4 <- fig_sun.z0 +
  geom_rect(data=plant.guide.spct,
            aes(xmin = wl.low, xmax = wl.high,
                ymin = y + 0.85, ymax = y + 0.9,
                y = 0, fill=wb.color),
            color = "white") +
  scale_fill_identity()

fig_sun.z4
```



We add text labels on top of the guide, and make the rectangle borders and text white to make the separation between the different 'invisible' wavebands clear. As we are adding labels, the 'guide' or key becomes redundant and we remove it by adding `guide="none"` to the fill scale.

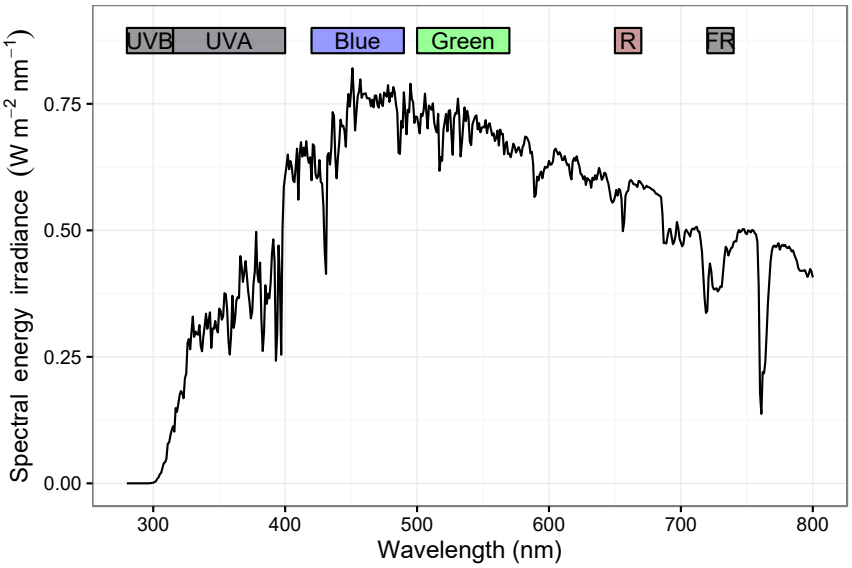
```
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z5 <- fig_sun.z0 +
  geom_rect(data=plant.guide.spct,
            aes(xmin = wl.low, xmax = wl.high,
                ymin = y + 0.85, ymax = y + 0.9,
                y = 0, fill=wb.color),
            color = "white") +
  geom_text(data=plant.guide.spct,
            aes(y = y + 0.875, label = as.character(wb.f)),
            color = "white", size=4) +
  scale_fill_identity()

fig_sun.z5
```



Here we add `alpha` or transparency to make the colours paler, and use black text and lines.

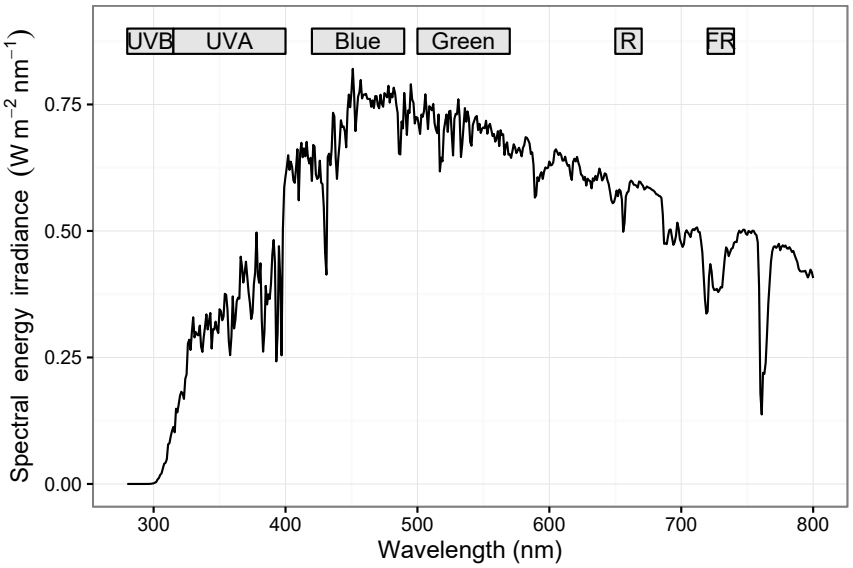
```
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z6 <- fig_sun.z0 +
  geom_rect(data=plant.guide.spct,
       aes(xmin = wl.low, xmax = wl.high,
           ymin = y + 0.85, ymax = y + 0.9,
           y = 0, fill=wb.color),
       color = "black", alpha=0.4) +
  geom_text(data=plant.guide.spct,
       aes(y = y + 0.875, label = as.character(wb.f)),
       color = "black", size=4) +
  scale_fill_identity()
```

```
fig_sun.z6 + theme_bw()
```



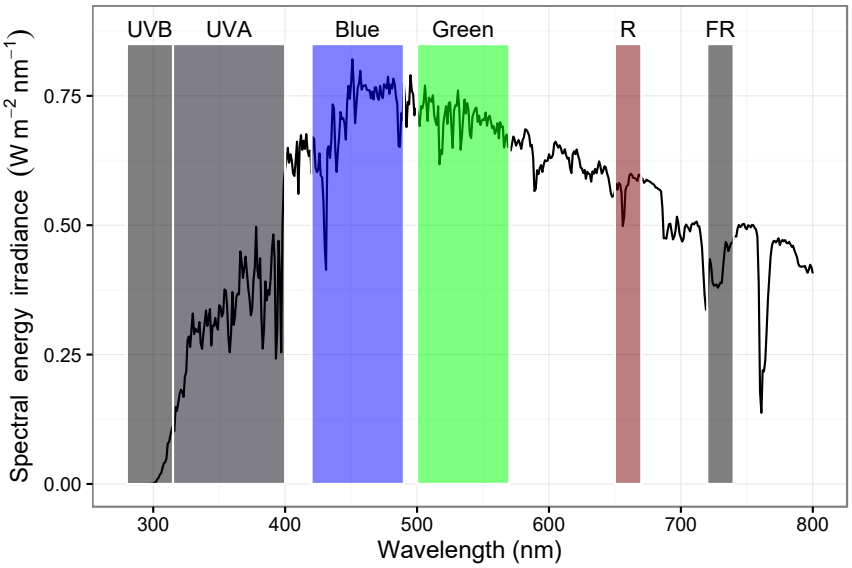
We change the guide so that all rectangles are filled with the same shade of grey by moving `fill` out of `aes` and setting it to a constant.

```
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z7 <- fig_sun.z0 +
  geom_rect(data=plant.guide.spct,
            aes(xmin = wl.low, xmax = wl.high,
                ymin = y + 0.85, ymax = y + 0.9,
                y = 0),
            color = "black", fill="grey90") +
  geom_text(data=plant.guide.spct,
            aes(y = y + 0.875, label = as.character(wb.f)),
            color = "black", size=4)

fig_sun.z7 + theme_bw()
```



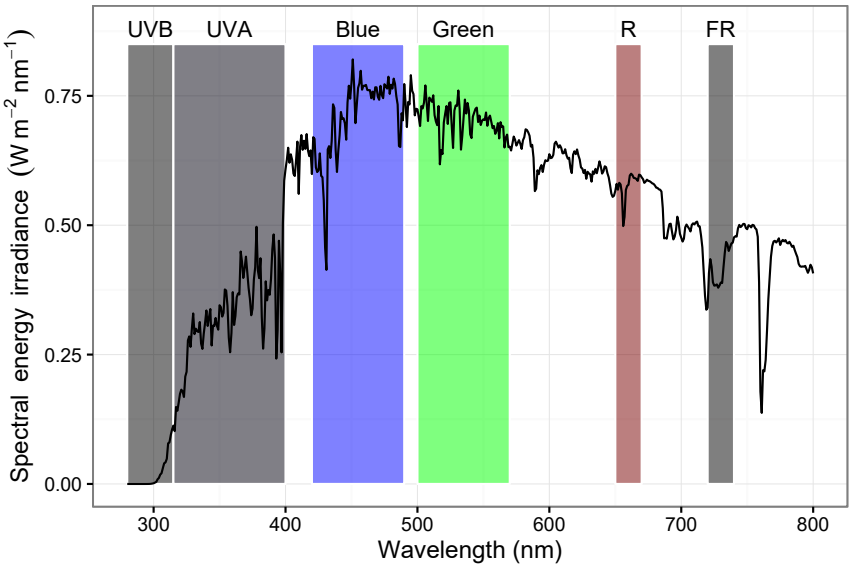
We can obtain annotations similar to those in ?? in page ?? created with `annotate_waveband` using geoms.

```
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z8 <- fig_sun.z0 +
  geom_rect(data=plant.guide.spct,
       aes(xmin = wl.low, xmax = wl.high,
           ymin = y, ymax = y + 0.85,
           y = 0, fill=wb.color),
       color = "white", alpha=0.5) +
  geom_text(data=plant.guide.spct,
       aes(y = y + 0.88, label = as.character(wb.f)),
       color = "black") +
  scale_fill_identity()

fig_sun.z8 + theme_bw()
```



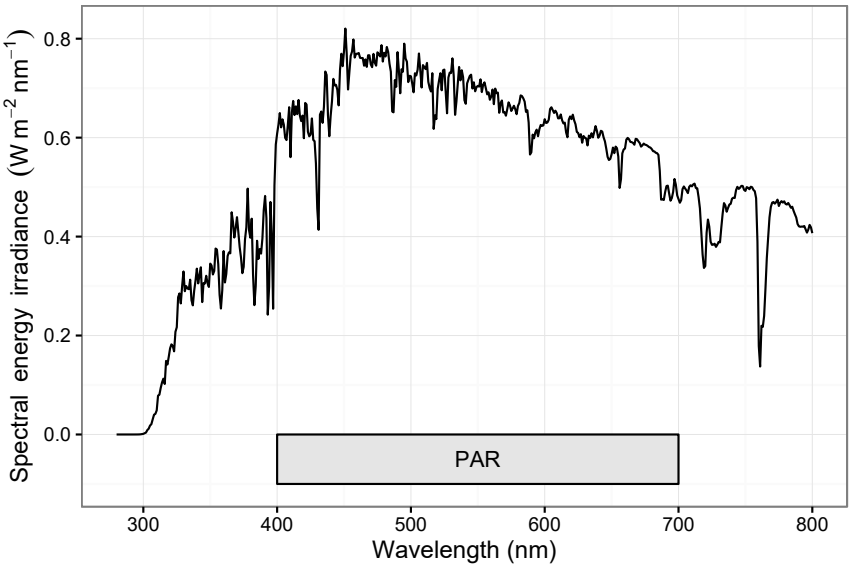
The example above can be improved by changing the order in which the geoms are added. In the plot above we can see that the rectangles are plotted on top of the line for the spectral irradiance. By changing the order we obtain a better plot.


```
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z8a <-
  ggplot(data=sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_rect(data=plant.guide.spct,
       aes(xmin = wl.low, xmax = wl.high,
           ymin = y, ymax = y + 0.85,
           y = 0, fill=wb.color),
       color = "white", alpha=0.5) +
  scale_fill_identity() +
  geom_text(data=plant.guide.spct,
       aes(y = y + 0.88, label = as.character(wb.f)),
       color = "black") +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.z8a + theme_bw()
```



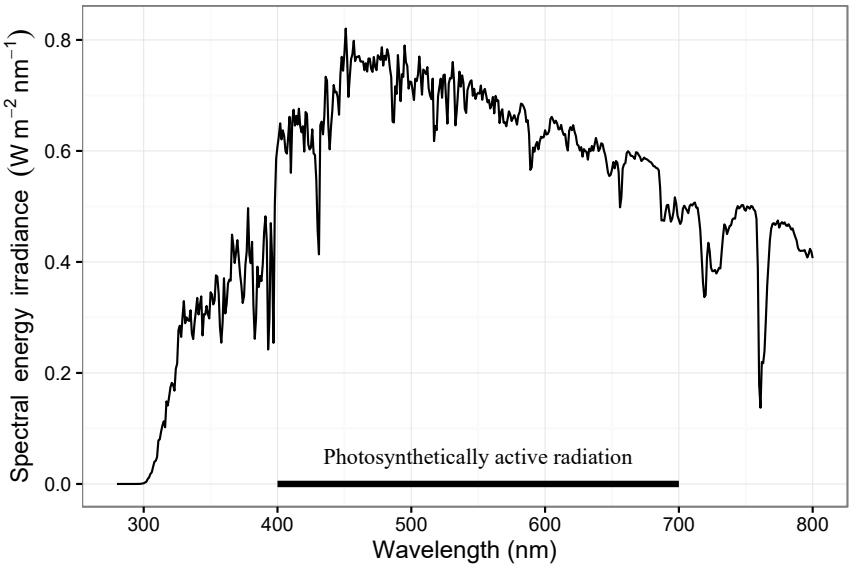
In the examples above we used predefined lists of wavebands, but one can, of course, use any list of waveband definitions, for example explicitly created with `list` and `new_waveband`, or `list` and any combination of user-defined and predefined wavebands. Even single waveband definitions are allowed.

```
par.guide.spct <- wb2rect_spct(PAR())

fig_sun.z9 <- fig_sun.z0 +
  geom_rect(data=par.guide.spct,
            aes(xmin = wl.low, xmax = wl.high,
                ymin = y - 0.1, ymax = y,
                y = 0),
            color = "black", fill="grey90") +
  geom_text(data=par.guide.spct,
            aes(y = y - 0.05, label = as.character(wb.f)),
            color = "black")

fig_sun.z9 + theme_bw()
```



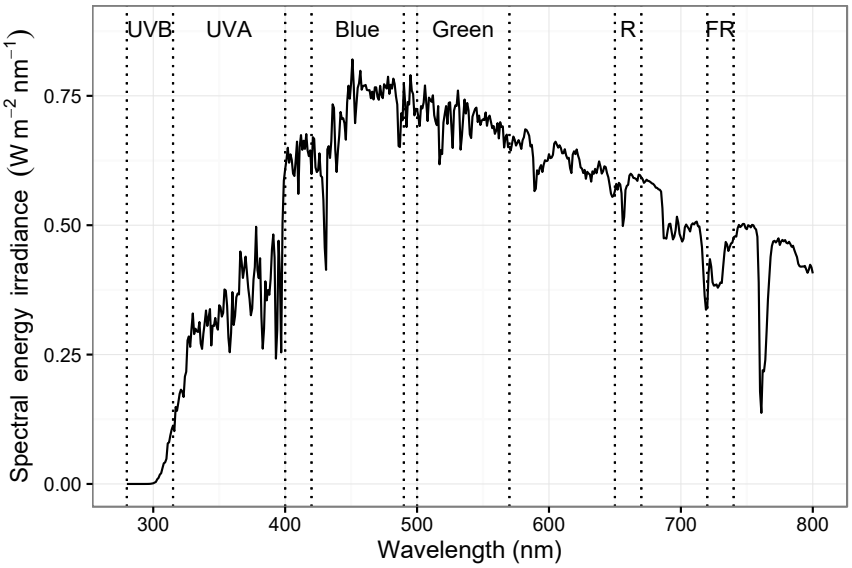
We can also use `geom_segment` to draw lines, including arrows. In this example we also set a different font `family` and label text. We can replace the label text which is by default obtained from the waveband definition by assigning a name to the waveband as member of the list. We use single quotes so that the long name containing space characters is accepted by `list`.

```
par.guide1.spct <-
  wb2rect_spct(list('Photosynthetically active radiation' = PAR()))

fig_sun.z10 <- fig_sun.z0 +
  geom_segment(data=par.guide1.spct,
       aes(x = wl.low, xend = wl.high,
           y = y, yend = y),
       size = 1.5, color = "black") +
  geom_text(data=par.guide1.spct,
       aes(y = y + 0.05, label = as.character(wb.f)),
       color = "black", family="serif")

fig_sun.z10 + theme_bw()
```



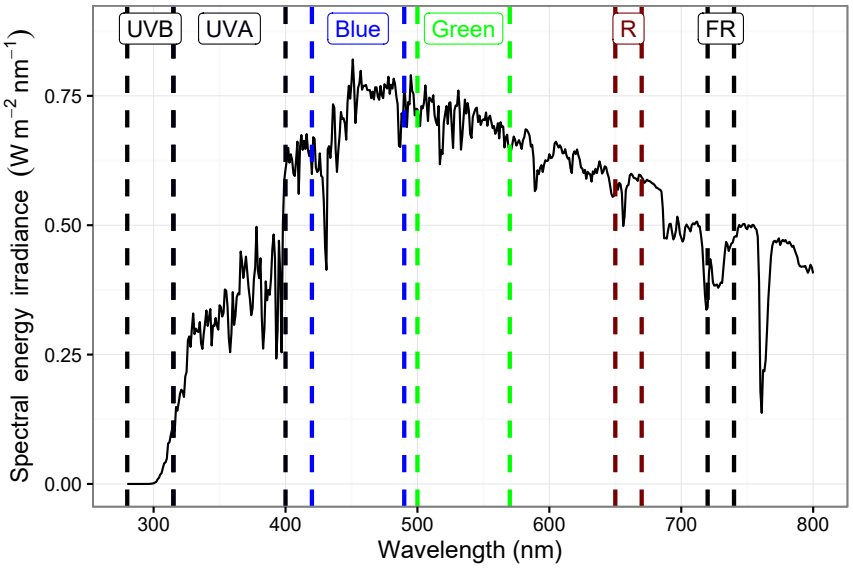
In this section we have used until now function `wb2rect_spct` to create 'spectral' annotation data from waveband definitions. Two other functions are available, that are needed or easier to use in some cases. One such case is when we have a list of wavebands and we would like to mark their boundaries with vertical lines. How to do this with `annotate` and `range` was show earlier in this chapter, but this can become tedious when we have several wavebands. Here we show an alternative approach.

```
plant.boundaries.spct <- wb2spct(Plant_bands())
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z11 <- fig_sun.z0 +
  geom_vline(data=plant.boundaries.spct,
             aes(xintercept = w.length),
             linetype = "dotted") +
  geom_text(data=plant.guide.spct,
       aes(y = y + 0.88, label = as.character(wb.f)),
       color = "black")

fig_sun.z11 + theme_bw()
```



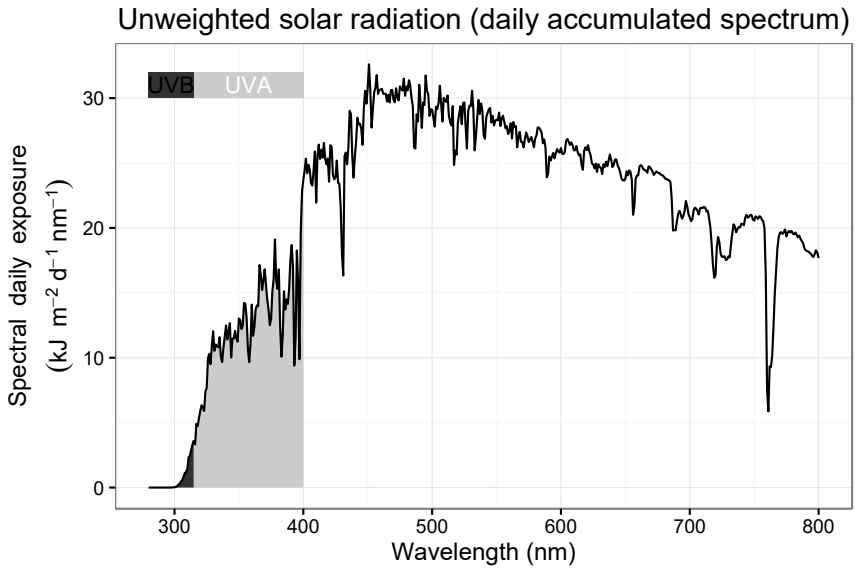
Function `wb2tagged_spct` returns the same data as `wb2spct` but 'tagged'. As shown in the next code chunk, tagging allows us to use waveband-dependent colours to the vertical lines.

```
plant.boundaries.spct <- wb2tagged_spct(Plant_bands())
plant.guide.spct <- wb2rect_spct(Plant_bands())

fig_sun.z12 <- fig_sun.z0 +
  geom_vline(data=plant.boundaries.spct,
             aes(xintercept = w.length, color=wb.color),
             size=1, linetype="dashed") +
  geom_label(data=plant.guide.spct,
       aes(y = y + 0.88, label = as.character(wb.f), color=wb.color),
       size=4) +
  scale_color_identity()

fig_sun.z12 + theme_bw()
```



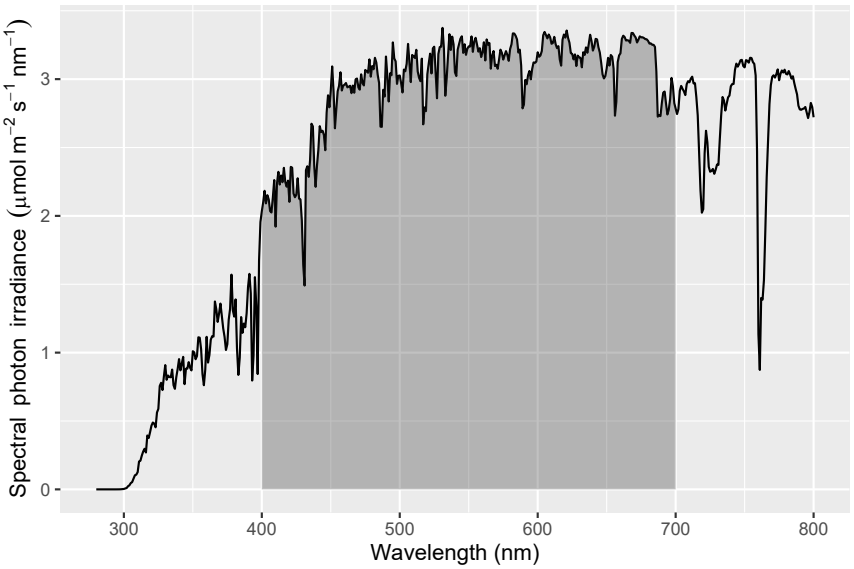
Of course it is possible to combine tagged data spectra and tagged spectra created from wavebands. The tagging is consistent, so, as demonstrated in the next figure, the same aesthetic 'link' works for both spectra. In this case the fill scale and the setting of fill to `wb.f` work across different 'data' and yield a consistent look. This figure also shows that when assigning a constant to an aesthetic, it is possible to use a vector, which in the present example, saves us some work compared to adding a column to the data and using an identity scale. Contrary to earlier examples where we have added layers to a previously saved plot, here we show the whole code needed to build the figure.

```
my.sun.spct <- tag(sun.daily.spct, list(UVB(), UVA()))
annotation.spct <- wb2rect_spct(list(UVB(), UVA()))
fig_sun.uv1 <- ggplot(my.sun.spct,
                      aes(x=w.length,
                          y=s.e.irrad * 1e-3,
                          fill=wb.f)) +
  scale_fill_grey(na.value=NA, guide="none") +
  geom_area() + geom_line() +
  labs(x = "Wavelength (nm)",
       y =  expression(atop(Spectral~~daily~~exposure,
                            (kJ~~m^{-2}~d^{-1}~nm^{-1}))),
       fill = "",
       title =
   "Unweighted solar radiation (daily accumulated spectrum)") +
  geom_rect(data=annotation.spct,
            aes(xmin=wl.low, xmax=wl.high, ymin=30, ymax=32)) +
  geom_text(data=annotation.spct,
            aes(label=as.character(wb.f), y=31),
            color=c("black", "white"), size=4) +
  theme_bw()

fig_sun.uv1
```

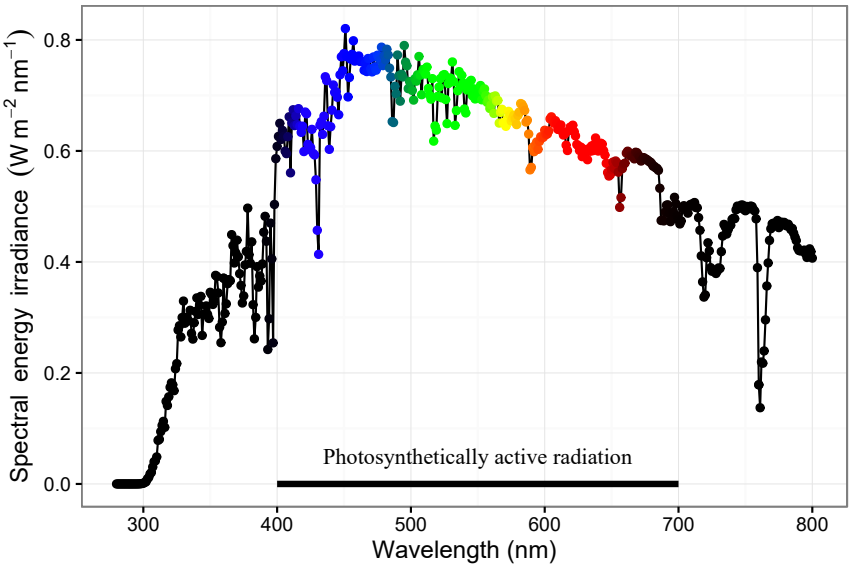


Possible variations are almost endless, so we invite the reader to continue exploring how the functions from package 'photobiology' can be used together with those from package 'ggplot2', to obtain beautiful plots of spectra. As an example here we show new versions of two plots from the previous section, one using a filled area to label the PAR region, and another one using symbols with colours according to their wavelength, to which we add a guide for PAR.

```
par <- q_irrad(sun.spct, PAR()) * 1e6

fig_sun.tgrect1 <-
  ggplot(data=par.sun.spct,
         aes(x=w.length, y=s.q.irrad * 1e6)) +
  geom_line() +
  geom_area(color=NA, alpha=0.3, aes(fill=wb.f))  +
  scale_fill_grey(na.value=NA, guide="none") +
  labs(
    y = ylab_umol,
    x = "Wavelength (nm)") #+
#  stat_wb_irrad(w.band = PAR())

fig_sun.tgrect1
```




```
par.guide.spct <-
  wb2rect_spct(list('Photosynthetically active radiation' = PAR()))

fig_sun.tgrect2 <-
  ggplot(data=tg.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  scale_color_identity() +
  geom_point(aes(color=wl.color))  +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)") +
  geom_segment(data=par.guide.spct,
       aes(x = wl.low, xend = wl.high, y = y, yend = y),
       size = 1.5, color = "black") +
  geom_text(data=par.guide.spct,
       aes(y = y + 0.05, label = as.character(wb.f)),
       color = "black", family="serif")

fig_sun.tgrect2 + theme_bw()
```

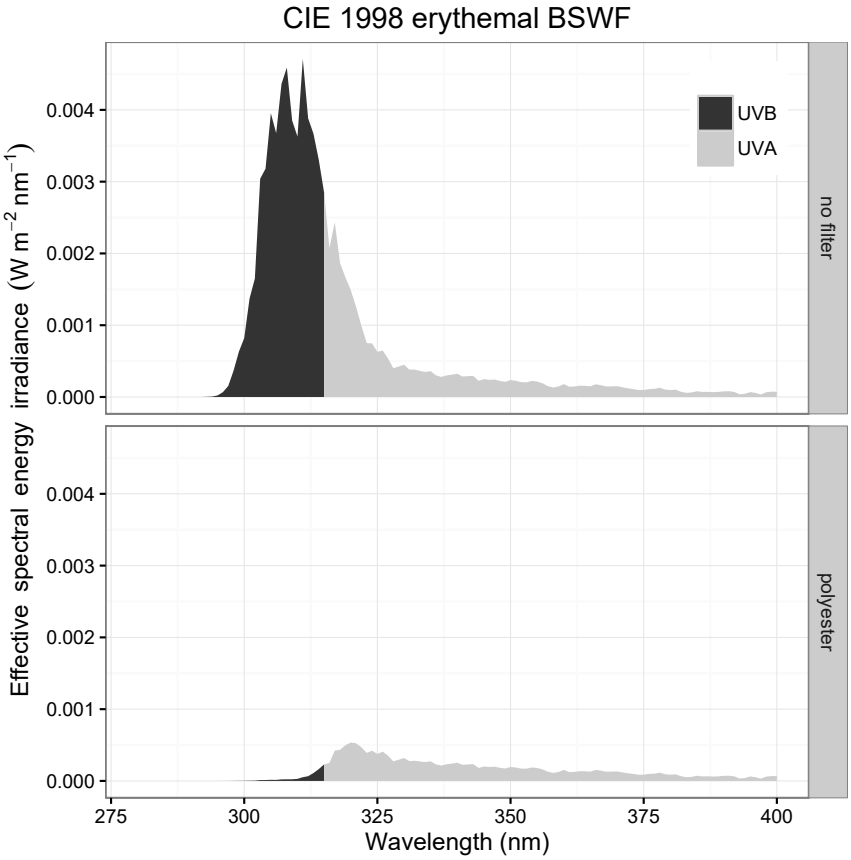


16.6 Plotting the result of operations on spectral data

16.6.1 Task: plotting effective spectral irradiance

This task is here simply to show that there is nothing special about plotting spectra based on calculations, and that one can combine different functions to get the job done. We also show how to 'row bind' spectra for plotting, in this case to make it easy to use facets.

```
sun.eff.cie.nf.spct <-
    tag(sun.spct * CIE(), UV_bands())
sun.eff.cie.pe.spct <-
    tag(sun.spct * polyester.spct * CIE(), UV_bands())
sun.eff.cie.spct <-
    rbindspct(list('no filter' = sun.eff.cie.nf.spct,
                   'polyester' = sun.eff.cie.pe.spct),
              idfactor = "filter")

fig_sun.cie0 <-
  ggplot(data=sun.eff.cie.spct, aes(x=w.length, y=s.e.irrad, fill=wb.f)) +
  scale_fill_grey() +
  geom_area() +
  labs(x = xlab_nm,
       y = expression(Effective~~spectral~~energy~~irradiance~~(W~m^{-2}~nm^{-1})),
       title = "CIE 1998 erythemal BSWF") +
  facet_grid(filter~.) +
  labs(fill="") +
  xlim(NA, 400) +
  theme_bw() +
  theme(legend.position=c(0.90, 0.9))

fig_sun.cie0
```



There is one warning issued for each panel, as the use of `xlim` discards 400 observations for wavelengths longer than 400 (nm). One should be aware that these are estimated values and in practice stray light reduces the efficiency of the filters for blocking radiation, and the amount of stray light depends on many factors including the relative positions of plants, filter and sun.

A couple of details need to be remembered: the tagging has to be done before row-binding the spectra, as `tag` works only on spectra that have unique values for wavelengths and discards 'repeated' rows if they are present. We use `theme(legend.position=c(0.90, 0.9))` to change where the legend or guide is positioned. In this case, we move the legend to a place within the plotting region. As we are using also `theme_bw()` which resets the legend position to the default, the order in which they are added is significant.

16.6.2 Task: making a bar plot of effective irradiance

In this task we aim at creating bar plots depicting the contributions of the UVB and UVA bands to the total erythemal effective irradiance in sunlight filtered with different plastic films. First we calculate the effective energy irradiance using the waveband definition for *erythemal* BSWF (CIE98) separately for the estimated solar spectral irradiance under each filter type.

```
cie.nf.irrad <- e_irrad(sun.spct * CIE(),
                        list(UVB(), UVA()))
cie.pe.irrad <- e_irrad(sun.spct * polyester.spct * CIE(),
                        list(UVB(), UVA()))
```

We assemble a data table by concatenating the irradiance and adding factors for filter type and wave bands. When defining the factors, we use `levels` to make sure that the levels are ordered as we would like to plot them.

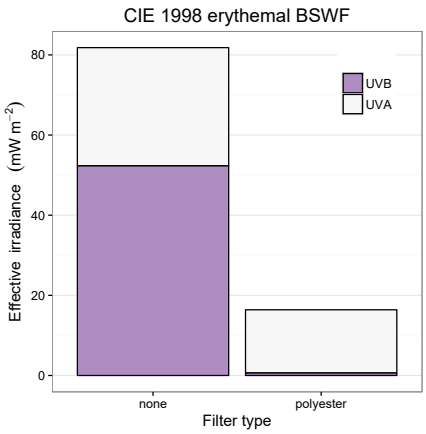
```
cie.dt <- data_frame(
  cie.irrad = c(cie.nf.irrad, cie.pe.irrad),
  filter = factor(rep(c('none', 'polyester'), c(2,2)),
                  levels=c('none', 'polyester')),
  w.band = factor(rep(c('UVB', 'UVA'), 2),
                  levels=c('UVB', 'UVA')) )
```

Now we plot stacked bars using `geom_bar`, however as the default `stat` of this `geom` is not suitable for our data, we specify `stat="identity"` to have the data plotted as is. We set a specific palette for fill, and add a black border to the bars by means of `color="black"`, we remove the grid lines corresponding to the x-axis, and also position the legend within the plotting region.

```
cie.dt
```

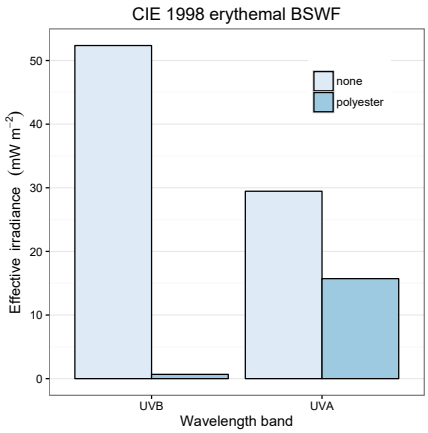
```
## # A tibble: 4 x 3
##      cie.irrad    filter w.band
##          <dbl>    <fctr> <fctr>
## 1 0.0523585311      none    UVB
## 2 0.0294572964      none    UVA
## 3 0.0006758325 polyester    UVB
## 4 0.0157202386 polyester    UVA
```

```
fig_cie_bars0 <- ggplot(data=cie.dt,
                        aes(y = cie.irrad * 1e3,
                            x = filter,
                            fill = w.band)) +
  scale_fill_brewer(palette="PRGn") +
  geom_bar(stat="identity", colour="black") +
  labs(x = "Filter type",
       y = expression(Effective~~irradiance~~~(mW~m^{-2})),
       title = "CIE 1998 erythemal BSWF",
       fill = "") +
  theme_bw(13) +
  theme(legend.position=c(0.85, 0.85)) +
  theme(panel.grid.minor.x=element_blank(),
        panel.grid.major.x=element_blank())

fig_cie_bars0
```



The figure above is good for showing the relative contribution of UVB and UVA radiation to the total effect, and the size of the total effect. On the other hand if we would like to show how much the effective irradiance in the UVB and UVA decreases under each of the filters is better to avoid stacking of the bars, plotting them side by side using `position=position_dodge()`. In addition we swap the aesthetics to which the two factors are linked.

```
fig_cie_bars1 <- ggplot(data=cie.dt,
                        aes(y = cie.irrad * 1e3,
                            x = w.band,
                            fill=filter)) +
  geom_bar(stat="identity",
           position=position_dodge(),
           color="black") +
  scale_fill_brewer() +
  labs(x = "Wavelength band",
       y = expression(Effective~~irradiance~~~(mW~m^{-2})),
       title = "CIE 1998 erythemal BSWF",
       fill = "") +
  theme_bw() +
  theme(legend.position=c(0.80, 0.85)) +
  theme(panel.grid.minor.x=element_blank(),
        panel.grid.major.x=element_blank())

fig_cie_bars1
```



16.6.3 Task: plotting a spectrum using colour bars

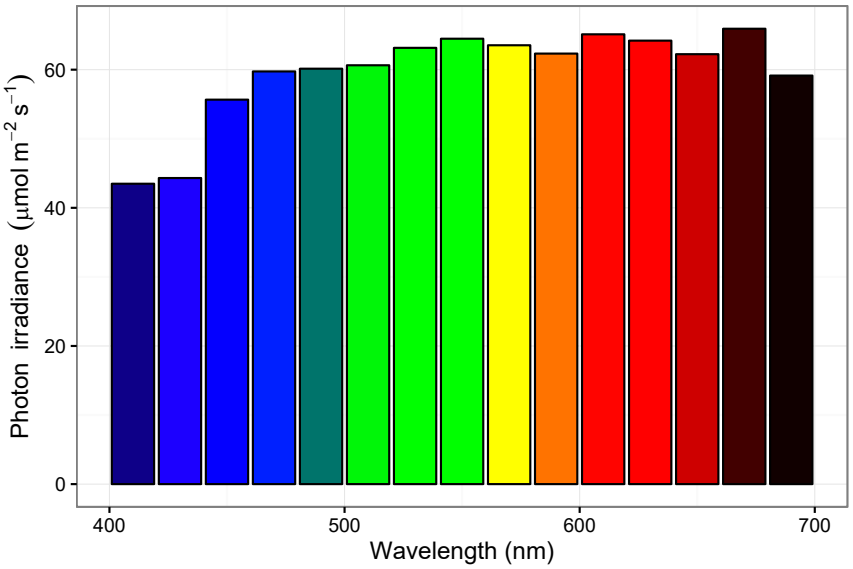
We show now the last example, related to the ones above, but creating a bar plot with more bars. First we calculate photon irradiance for different equally spaced bands within PAR using function `split_bands`. The code is written so that by changing the first two lines you can adjust the output.

```
wl.range <- range(PAR())
num.bands <- 15
many.bands <- split_bands(wl.range, length.out=num.bands)
w.length <- numeric(num.bands)
wb.name <- wb.color <- character(num.bands)

for (i in 1:num.bands) {
  w.length[i] <- midpoint(many.bands[[i]])
  wb.color[i] <- color(many.bands[[i]], type="CMF")
  wb.name[i] <- labels(many.bands[[i]])[["name"]]
}

q.irrad.bands.sun <- q_irrad(sun.spct, many.bands)
q.irrad.sun.spct <- data_frame(q.irrad = q.irrad.bands.sun,
                               w.length = w.length,
                               wb.color = wb.color,
                               wb.name = wb.name)
```

Now we can plot the data as bars, filling each bar with the corresponding colour. In this case we plot the bars using a continuous variable, wavelength, for the x-axis.

```
fig_qirrad_bar <- ggplot(data=q.irrad.sun.spct,
                         aes(y = q.irrad * 1e6,
                             x = w.length,
                             fill=as.character(wb.color))) +
  geom_bar(stat="identity",
           color="black") +
  scale_fill_identity(guide="none") +
  labs(x = xlab_nm,
       y = expression(Photon~~irradiance~~(mu*mol~m^{-2}~s^{-1})),
       fill = "") +
  theme_bw()
```

```
fig_qirrad_bar
```



In the case of the example spectrum with equal wavelength steps, one could have directly summed the values, however, the approach shown here is valid for any type of spacing of the values along the wavelength axis, including variable one, like is the case for array spectrometers.

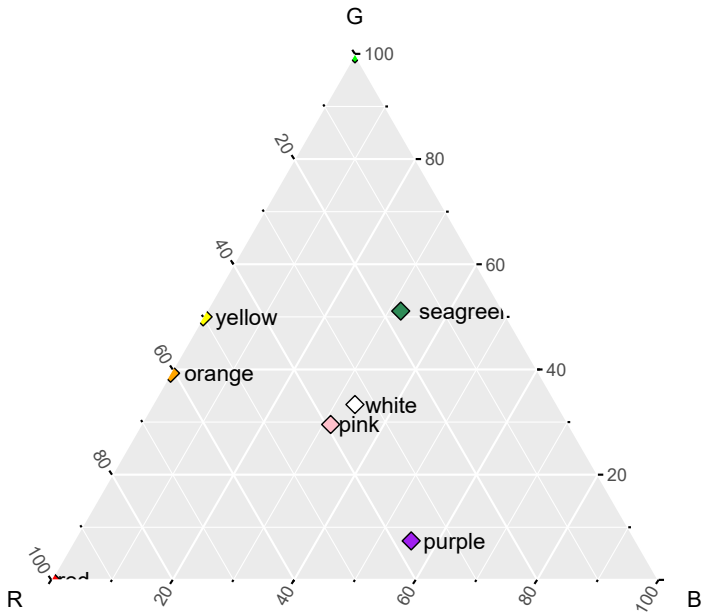
16.7 Task: plotting colours in Maxwell's triangle

16.7.1 Human vision: RGB

Given a color definition, we can convert it to RGB values by means of R's function `col2rgb`. We can obtain a color definition for monochromatic light from its wavelength with function `w_length2rgb` (see section ??), from a waveband with function `color` (see section ??), for a wavelength range with `w_length_range2rgb` (see section ??), and from a spectrum with function `s_e_irrad2rgb` (see section ??). The RGB values can be used to locate the position of any colour on Maxwell's triangle, given a set of chromaticity coordinates defining the triangle. In the first example we use some of R's predefined colors. We use the function `ggtern` from the package of the same name. It is based on `ggplot` and to produce a ternary diagram we need to use `ggtern` instead of `ggplot`. Geometries, aesthetics, stats and faceting function normally in most cases. Of course, being a ternary plot, the aesthetics `x`, `y`, and `z` should be all assigned to variables in the data.

```
colours <- c("red", "green", "yellow", "white",
             "orange", "purple", "seagreen", "pink")
rgb.values <- col2rgb(colours)
test.data <- data.frame(colour=colours,
                        R=rgb.values[1, ],
```

```
                        G=rgb.values[2, ],
                        B=rgb.values[3, ])
maxwell.tern <- ggtern(data=test.data,
                       aes(x=R, y=G, z=B, label=colour, fill=colour)) +
                       geom_point(shape=23, size=3) +
  geom_text(hjust=-0.2) +
  labs(x = "R", y="G", z="B") + scale_fill_identity()
maxwell.tern
```



16.8 Honey-bee vision: GBU

In this case we start with the spectral responsiveness of the photoreceptors present in the eyes of honey bees. Bees, as humans have three photoreceptors, but instead of red, green and blue (RGB), bees see green, blue and UV-A (GBU). To plot colours seen by bees one can still use a ternary plot, but the axes represent different photoreceptors than for humans, and the colour space is shifted towards shorter wavelengths.

The calculations we will demonstrate here, in addition are geared to compare a background to a foreground object (foliage vs. flower). We have followed xxxxx **chitka?** in this example, but be aware that calculations presented in this reference do not match the equations presented. In the original published example, the calculations have been simplified by leaving out $\delta\lambda$. Although not affecting the final result for their ex-

ample, intermediate results are different (wrong?). We have further generalized the calculations and equations to make the calculations also valid for spectra measured using $\delta\lambda$ that itself varies along the wavelength axis. This is the usual situation with array spectrometers, nowadays frequently used when measuring reflectance.

The assessment of the perceived 'colour difference' between background and foreground objects requires taking into consideration several spectra: the incident 'light' spectrum, the reflectance spectra of the two objects, and the sensitivity spectra of three photoreceptors in the case of trichromic vision. In addition to these data, we need to take into consideration the shape of the dose response of the photoreceptors.

```
try(detach(package:ggspectra))
try(detach(package:ggtern))
try(detach(package:ggplot2))
try(detach(package:gridExtra))
try(detach(package:photobiologyFilters))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

17

Radiation physics

17.1 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(ggplot2)
library(ggspectra)
library(photobiology)
library(photobiologyFilters)
```

17.2 Introduction

17.3 Task: black body emission

The emitted spectral radiance (L_s) is described by Planck's law of black body radiation at temperature T, measured in degrees Kelvin (K):

$$L_s(\lambda, T) = \frac{2hc^2}{\lambda^5} \cdot \frac{1}{e^{(hc/k_B T\lambda)} - 1} \tag{17.1}$$

with Boltzmann's constant $k_B = 1.381 \times 10^{-23}$ $\mathrm{J\,K^{-1}}$, Planck's constant $h = 6.626 \times 10^{-34}$ $\mathrm{J\,s}$ and speed of light in vacuum $c = 2.998 \times 10^{8}$ $\mathrm{m\,s^{-1}}$.

We can easily define an R function based on the equation above, which returns $\mathrm{W\,sr^{-1}\,m^{-3}}$:

```
h <- 6.626e-34 # J s-1
c <- 2.998e8 # m s-1
kB <- 1.381e-23 # J K-1
black_body_spectrum <- function(w.length, Tabs) {
  w.length <- w.length * 1e-9 # nm -> m
  ((2 * h * c^2) / w.length^5) *
    1 / (exp((h * c / (kB * Tabs * w.length))) - 1)
}
```

We can use the function for calculating black body emission spectra for different temperatures:

```
black_body_spectrum(500, 5000)

## [1] 1.212443e+13
```

The function is vectorised:

```
black_body_spectrum(c(300,400,500), 5000)

## [1] 3.354907e+12 8.759028e+12 1.212443e+13
```

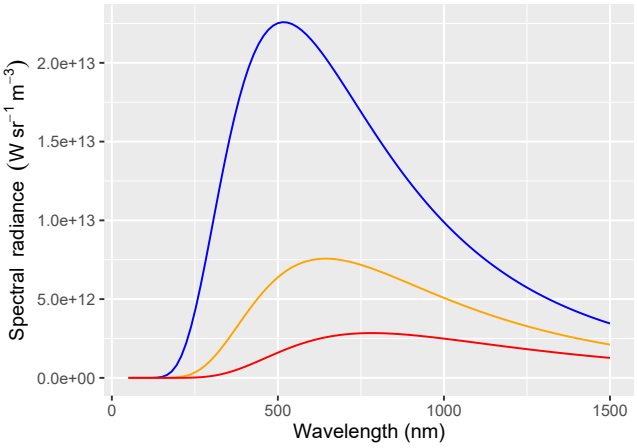
```
black_body_spectrum(500, c(4500,5000))

## [1] 6.387979e+12 1.212443e+13
```

We aware that if two vectors are supplied, then the elements in each one are matched and recycled[1]:

```
black_body_spectrum(c(500, 500, 600, 600), c(4500,5000)) # tricky!

## [1] 6.387979e+12 1.212443e+13 7.474587e+12
## [4] 1.277769e+13
```

We can use the function defined above for plotting black body emission spectra for different temperatures. We use 'ggplot2' and directly plot a function using `stat_function`, using `args` to pass the additional argument giving the absolute temperature to be used. We plot three lines using three different temperatures (5600 K, 4500 K, and 3700 K):

```
ggplot(data=data.frame(x=c(50,1500)), aes(x)) +
  stat_function(fun=black_body_spectrum,
                args = list(Tabs=5600),
                colour="blue") +
  stat_function(fun=black_body_spectrum,
                args = list(Tabs=4500),
                colour="orange") +
  stat_function(fun=black_body_spectrum,
                args = list(Tabs=3700),
                colour="red") +
  labs(y=expression(Spectral~~radiance~~(W~sr^-1~m^-3)),
       x="Wavelength (nm)")
```



[1] Exercise: calculate each of the four values individually to work out how the two vectors are being used.

Wien's displacement law, gives the peak wavelength of the radiation emitted by a black body as a function of its absolute temperature.

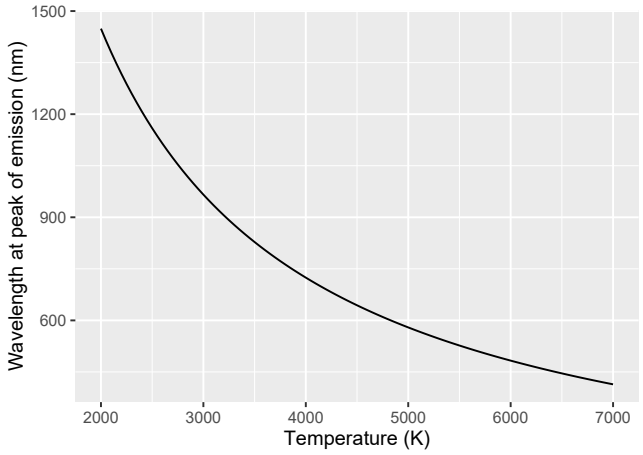
$$\lambda_{max} \cdot T = 2.898 \times 10^6 \,\mathrm{nm\,K} \tag{17.2}$$

A function implementing this equation takes just a few lines of code:

```
k.wein <- 2.8977721e6 # nm K
black_body_peak_wl <- function(Tabs) {
  k.wein / Tabs
}
```

It can be used to plot the temperature dependence of the location of the wavelength at which radiance is at its maximum:

```
ggplot(data=data.frame(Tabs=c(2000,7000)), aes(x=Tabs)) +
  stat_function(fun=black_body_peak_wl) +
  labs(x="Temperature (K)",
       y="Wavelength at peak of emission (nm)")
```




```
try(detach(package:photobiologyFilters))
try(detach(package:ggspectra))
try(detach(package:photobiology))
try(detach(package:ggplot2))
```

Part IV

Data acquisition and exchange

18

Importing and exporting 'R' data

18.1 Packages used in this chapter

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

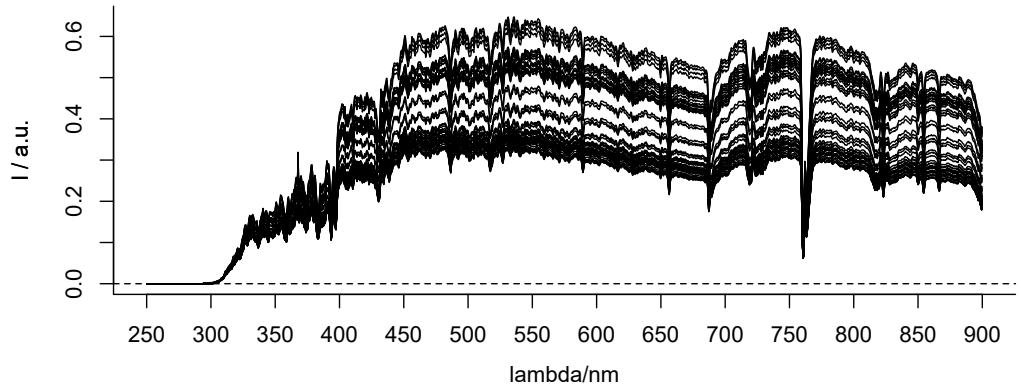
```
library(photobiology)
library(photobiologySun)
library(photobiologyWavebands)
library(photobiologyInOut)
library(lubridate)
library(ggplot2)
library(ggspectra)
library(hyperSpec)
library(colorSpec)
library(pavo)
library(fda)
library(fda.usc)
```

18.2 Package 'hyperSpec'

18.2.1 To 'hyperSpec'

Can export to `hyperSpec` objects only collections of spectra where all members have identical `w.length` vectors, as objects of class `hypeSpec` store a single vector of wavelengths for the whole collection of spectra. We use as example data `gap.mspct` from package 'photobiologySun'.

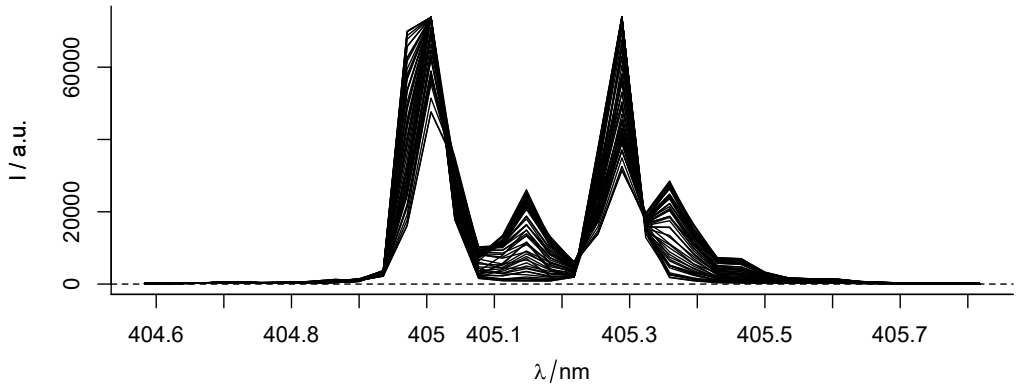
```
gap.hspct <- mspct2hyperSpec(gap.mspct, "s.e.irrad")

## Warning in .local(.Object, ...): Spectra in data are overwritten by argument spc.

class(gap.hspct)

## [1] "hyperSpec"
## attr(,"package")
## [1] "hyperSpec"

plot(gap.hspct)

## Warning in plotspc(x, ...): Number of spectra exceeds spc.nmax. Only the first 50
are plotted.
```



18.2.2 From 'hyperSpec'

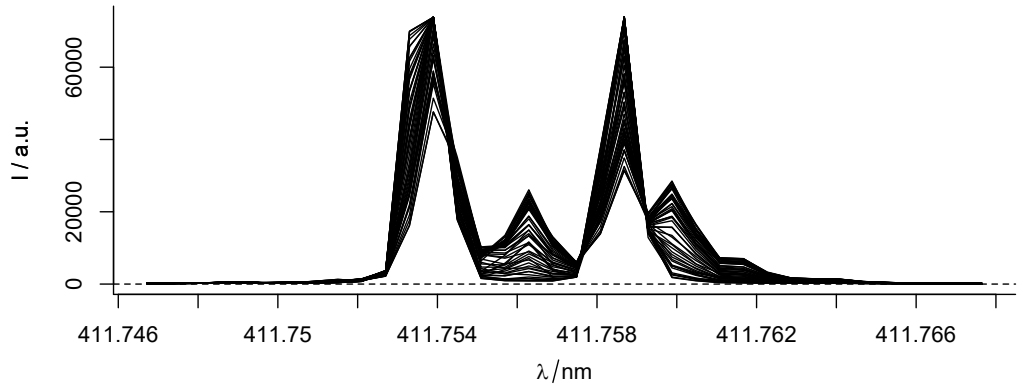
Can import only data with wavelength in nanometres. Other quantities and units are not supported by the 'photobiology' classes for spectral data. See package 'hyperSpec' vignette "laser" for details on the data and the conversion of the original wavelength units into nanometres.

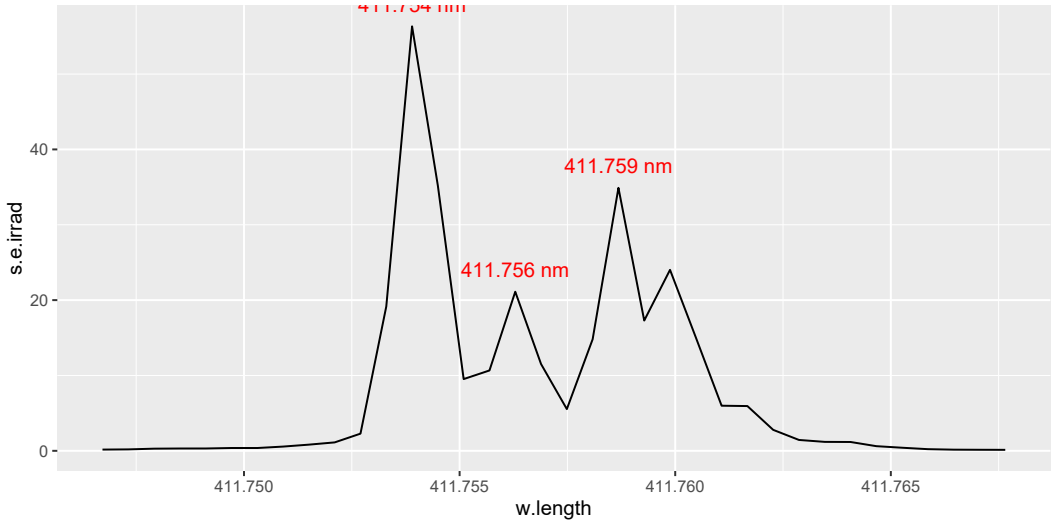
```
class(laser)

## [1] "hyperSpec"
## attr(,"package")
## [1] "hyperSpec"

laser

## hyperSpec object
##    84 spectra
##    2 data columns
##    36 data points / spectrum
## wavelength: lambda/nm [numeric] 404.5828 404.6181 ... 405.8176
## data:  (84 rows x 2 columns)
##    1. t: t / s [numeric] 0 2 ... 5722
##    2. spc: I / a.u. [matrix36] 164.650 179.724 ... 112.086

plot(laser)

## Warning in plotspc(x, ...): Number of spectra exceeds spc.nmax. Only the first 50
are plotted.
```



We assume here, that the quantity for the spectral emission of the laser is spectral *energy* irradiance, expressed in $\mathrm{mW\,cm^{-2}\,nm^{-1}}$. This is likely to be wrong but for the sake of showing how the conversion takes place is irrelevant. The parameter `multiplier` can be passed a numeric argument to rescale the original data. The default multiplier is 1.

```
wl(laser) <- list (
  wl = 1e7 / (1/405e-7 - wl (laser)),
  label = expression (lambda / nm)
)
laser

## hyperSpec object
##    84 spectra
##    2 data columns
##    36 data points / spectrum
## wavelength: lambda/nm [numeric] 411.7467 411.7473 ... 411.7677
## data:  (84 rows x 2 columns)
##    1. t: t / s [numeric] 0 2 ... 5722
##    2. spc: I / a.u. [matrix36] 164.650 179.724 ... 112.086

plot(laser)

## Warning in plotspc(x, ...): Number of spectra exceeds spc.nmax. Only the first 50
are plotted.

laser.mspct <-
  hyperSpec2mspct(laser, "source_spct", "s.e.irrad", multiplier = 1e-3)
ggplot(laser.mspct[[1]]) +
  geom_line() +
  stat_peaks(geom = "text", vjust = -1, label.fmt = "%.6g nm", color = "red")
```





18.3 Package 'colorSpec'

18.3.1 From 'colorSpec'

```
fluorescent.mspct <- colorSpec2mspct(Fs.5nm)
print(fluorescent.mspct, n = 3, n.members = 3)

## Object: source_mspct [12 x 1]
## --- Member: F1 ---
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm
## Time unit 1s
##
## # A tibble: 81 x 2
##   w.length s.e.irrad
```

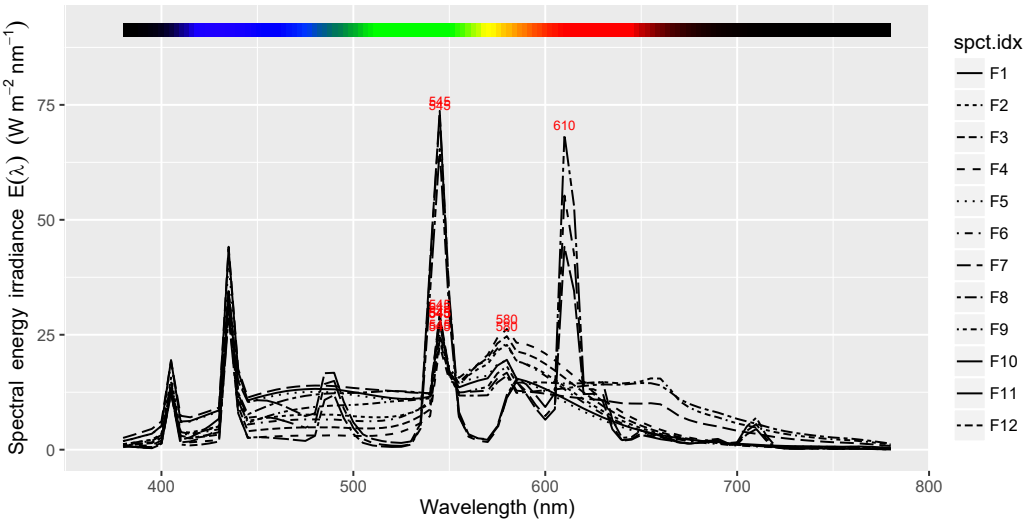
```
##      <dbl>     <dbl>
## 1      380      1.87
## 2      385      2.36
## 3      390      2.94
## # ... with 78 more rows
## --- Member: F2 ---
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm
## Time unit 1s
##
## # A tibble: 81 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1      380      1.18
## 2      385      1.48
## 3      390      1.84
## # ... with 78 more rows
## --- Member: F3 ---
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm
## Time unit 1s
##
## # A tibble: 81 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1      380      0.82
## 2      385      1.02
## 3      390      1.26
## # ... with 78 more rows
## ........................
## 9 other member spectra not shown
##
## --- END ---
```

```
colorSpec2mspct(Hoya)
```

```
## Object: filter_mspct [4 x 1]
## --- Member: R-60 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 x 2
##   w.length   Tfr
##      <dbl> <dbl>
## 1      300     0
## 2      310     0
## 3      320     0
## 4      330     0
## # ... with 42 more rows
## --- Member: G-533 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 x 2
##   w.length   Tfr
##      <dbl> <dbl>
## 1      300     0
## 2      310     0
## 3      320     0
## 4      330     0
```

```
## # ... with 42 more rows
## --- Member: B-440 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 x 2
##   w.length   Tfr
##       <dbl> <dbl>
## 1      300     0
## 2      310     0
## 3      320     0
## 4      330     0
## # ... with 42 more rows
## --- Member: LB-120 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 x 2
##   w.length     Tfr
##       <dbl>   <dbl>
## 1      300 0.00003
## 2      310 0.00580
## 3      320 0.08100
## 4      330 0.30400
## # ... with 42 more rows
##
## --- END ---
```

```
fluorescent.spct <- colorSpec2spct(Fs.5nm)
plot(fluorescent.spct, annotations = c("peaks", "color.guide")) + aes(linetype = spct.idx)
```

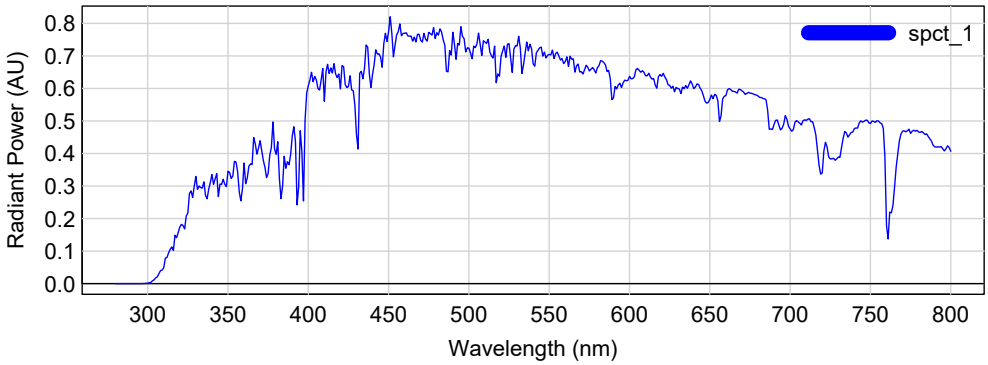



```
colorSpec2chroma_spct(xyz1931.5nm)

## Object: chroma_spct [81 x 4]
## Wavelength range 380 to 780 nm, step 5 nm
##
## # A tibble: 81 x 4
```

```
##         x     y      z w.length
## *   <dbl> <dbl>  <dbl>    <dbl>
## 1 0.0014 0e+00 0.0065      380
## 2 0.0022 1e-04 0.0105      385
## 3 0.0042 1e-04 0.0201      390
## 4 0.0076 2e-04 0.0362      395
## # ... with 77 more rows
```

18.3.2 To 'colorSpec'

```
sun.cspec <- spct2colorSpec(sun.spct)
plot(sun.cspec, col = "blue")
```




```
spct2colorSpec(yellow_gel.spct)

##
## colorSpec object.   The organization is 'vector'.  Object size is 11488 bytes.
## the object describes 1 transparent materials, and the quantity is 'transmittance'.
## Wavelength range: 190 to 800 nm.  Step size is 1 nm.
##
## 1 spectra
## 611 data points / spectrum
##
##   Material   Min    Max LambdaMax Integral
## 1   spct_1 1e-05 0.9025     768.5 260.3194
```

```
chroma_spct2colorSpec(beesxyzCMF.spct)

##
## colorSpec object.   The organization is 'matrix'.  Object size is 4128 bytes.
## the object describes a responder to light with 3 output channels, and the quantity is 'power->neural'.
## Wavelength range: 300 to 700 nm.  Step size is 5 nm.
##
```

```
## 3 spectra
## 81 data points / spectrum
##
##   Channel   Min Max LambdaMax E.response
## 1       x 0.000   1       340     68.965
## 2       y 0.000   1       435    103.850
## 3       z 0.006   1       560    135.620
```

18.4 Package 'pavo'

18.4.1 From 'pavo'

In this example we convert an `rspec` object from package 'pavo' into a collection of spectra and then we plot it with `ggplot` methods from package 'ggspectra' (an extension to 'ggplot2'). The data are the spectral reflectance of the plumage from seven different individual birds of the same species, measured in three different body parts.

```
data(sicalis)
class(sicalis)

## [1] "rspec"      "data.frame"

names(sicalis)

##  [1] "wl"     "ind1.C" "ind1.T" "ind1.B" "ind2.C"
##  [6] "ind2.T" "ind2.B" "ind3.C" "ind3.T" "ind3.B"
## [11] "ind4.C" "ind4.T" "ind4.B" "ind5.C" "ind5.T"
## [16] "ind5.B" "ind6.C" "ind6.T" "ind6.B" "ind7.C"
## [21] "ind7.T" "ind7.B"
```

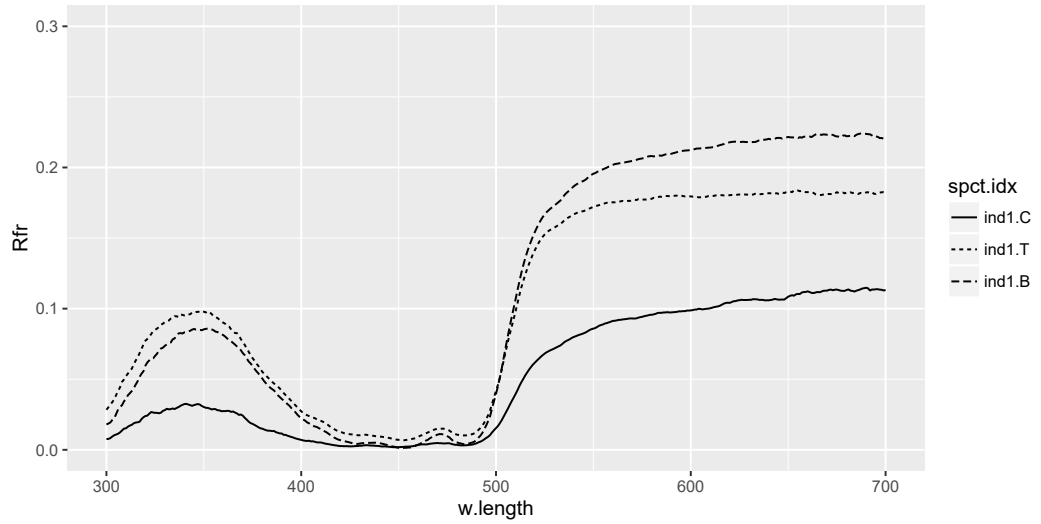
We convert the data into a collection of spectra, and calculate summaries for three spectra.

```
sicalis.mspct <- rspec2mspct(sicalis, "reflector_spct", "Rpc")
summary(sicalis.mspct[[1]])

## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
##     w.length        Rfr
##  Min.   :300   Min.   :0.001798
##  1st Qu.:400   1st Qu.:0.008288
##  Median :500   Median :0.031709
##  Mean   :500   Mean   :0.052848
##  3rd Qu.:600   3rd Qu.:0.098775
##  Max.   :700   Max.   :0.114807

summary(sicalis.mspct[[2]])

## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
##     w.length        Rfr
##  Min.   :300   Min.   :0.006783
```

```
##  1st Qu.:400   1st Qu.:0.030112
##  Median :500   Median :0.096994
##  Mean   :500   Mean   :0.105449
##  3rd Qu.:600   3rd Qu.:0.179691
##  Max.   :700   Max.   :0.183823

summary(sicalis.mspct[[3]])

## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
##     w.length        Rfr
##  Min.   :300   Min.   :0.001191
##  1st Qu.:400   1st Qu.:0.022293
##  Median :500   Median :0.085235
##  Mean   :500   Mean   :0.116253
##  3rd Qu.:600   3rd Qu.:0.212554
##  Max.   :700   Max.   :0.224162
```

We convert the subset of the collection corresponding to the first individual into a single spectra object for plotting with `ggplot`.

```
ggplot(rbindspct(sicalis.mspct[1:3])) +
  aes(linetype = spct.idx) +
  ylim(0,0.3) +
  geom_line()
```



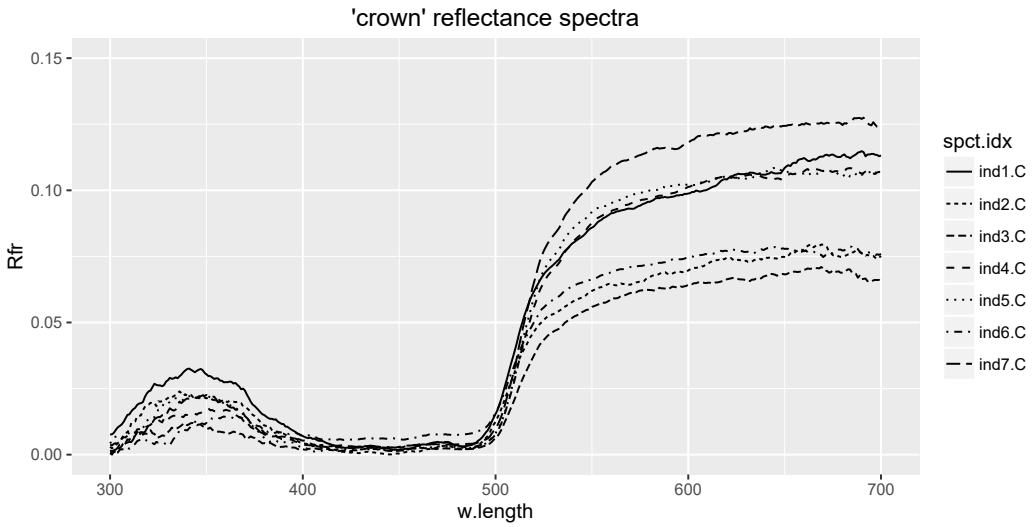
Here we extract the "crown" data from all individuals and plot these spectra in a single plot.

```
print(sicalis.mspct[c(TRUE, FALSE, FALSE)])

## Object: reflector_mspct [7 x 1]
## --- Member: ind1.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
```

```
##   w.length         Rfr
##      <dbl>       <dbl>
## 1      300 0.007594984
## 2      301 0.007727841
## 3      302 0.008288000
## 4      303 0.009414667
## # ... with 397 more rows
## --- Member: ind2.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
##   w.length         Rfr
##      <dbl>       <dbl>
## 1      300 0.002971167
## 2      301 0.002326722
## 3      302 0.003227833
## 4      303 0.003535167
## # ... with 397 more rows
## --- Member: ind3.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
##   w.length          Rfr
##      <dbl>        <dbl>
## 1      300 0.0005947619
## 2      301 0.0000000000
## 3      302 0.0011853968
## 4      303 0.0009427302
## # ... with 397 more rows
## --- Member: ind4.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
##   w.length         Rfr
##      <dbl>       <dbl>
## 1      300 0.003750159
## 2      301 0.003465714
## 3      302 0.004133333
## 4      303 0.004339333
## # ... with 397 more rows
## --- Member: ind5.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
##   w.length         Rfr
##      <dbl>       <dbl>
## 1      300 0.004225349
## 2      301 0.005361222
## 3      302 0.006554556
## 4      303 0.006816556
## # ... with 397 more rows
## --- Member: ind6.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
```

```
##   w.length          Rfr
##      <dbl>        <dbl>
## 1      300 0.0006326984
## 2      301 0.0006136508
## 3      302 0.0001934921
## 4      303 0.0008594921
## # ... with 397 more rows
## --- Member: ind7.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
##   w.length         Rfr
##      <dbl>       <dbl>
## 1      300 0.001680730
## 2      301 0.001043270
## 3      302 0.001702476
## 4      303 0.001939810
## # ... with 397 more rows
##
## --- END ---
```

```
ggplot(rbindspct(sicalis.mspct[c(TRUE, FALSE, FALSE)])) +
  aes(linetype = spct.idx) +
  ylim(0,0.15) +
  geom_line() +
  ggtitle("'crown' reflectance spectra")
```

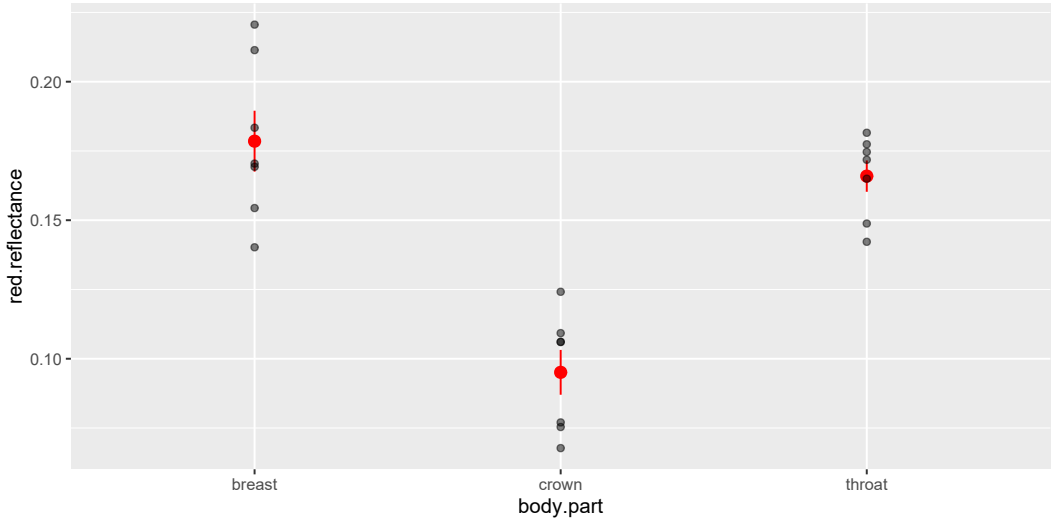


We calculate the mean reflectance in wavebands corresponding to ISO colors obtaining a data frame. We then add to this returned data frame a factor indicating the body parts.

```
refl.by.band <- reflectance(sicalis.mspct, w.band = list(Red(), Green(), Blue(), UVA()))
refl.by.band$body.part <- c("crown", "throat", "breast")
```

```
refl.red <- reflectance(sicalis.mspct, w.band = Red())
names(refl.red)[2] <- "red.reflectance"
```

```
refl.red$body.part <- c("crown", "throat", "breast")
ggplot(refl.red, aes(x = body.part, y = red.reflectance)) +
  stat_summary(fun.data = "mean_se", color = "red") +
  geom_point(alpha = 0.5)
```



18.5 Packages 'fda' and 'fda.usc'

Functional data analysis is a specialized method that can be used to compare and classify spectra. We here exemplify the selection of the 'deepest spectrum' from a collection of spectra. The data interconversion can be done with a simple function. Package 'fda' expects the spectra in a single matrix object, with each spectrum as a row. We will use once again `gap.mspct` for this example.

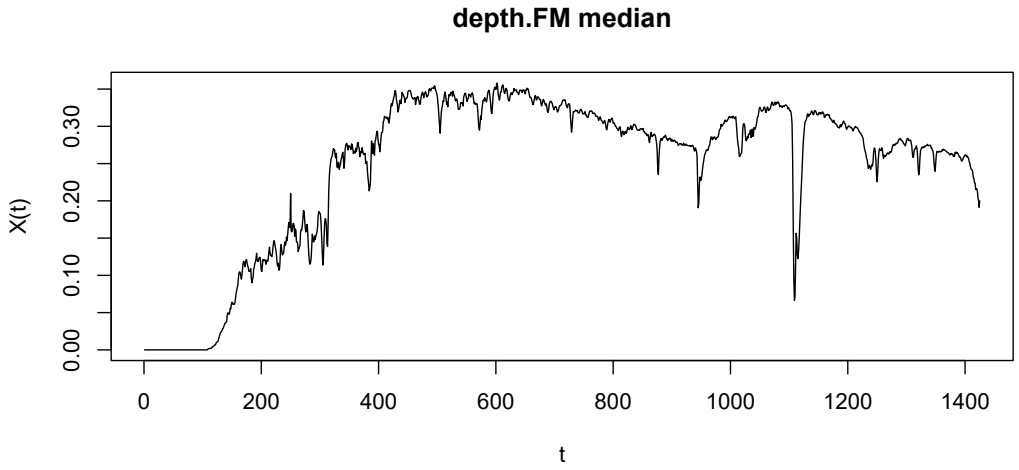
```
gap.mat <- mspct2mat(gap.mspct, "s.e.irrad", byrow = TRUE)
dim(gap.mat)

## [1]   72 1425

names(dimnames(gap.mat))

## [1] "spct"     "w.length"

# convert the matrix to fdata
gap.fdata <- fdata(gap.mat)
```

We search for "deepest curve" using different methods.

```
# Returns the deepest curve following FM criteria
func_med_FM <- func.med.FM(gap.fdata)
# Returns the deepest curve following mode criteria
func_med_mode <- func.med.mode(gap.fdata)
# Returns the deepest curve following RP criteria
func_med_RP <- func.med.RP(gap.fdata)
```

We plot using plot method from package 'fda'.

```
plot(func_med_FM)
```

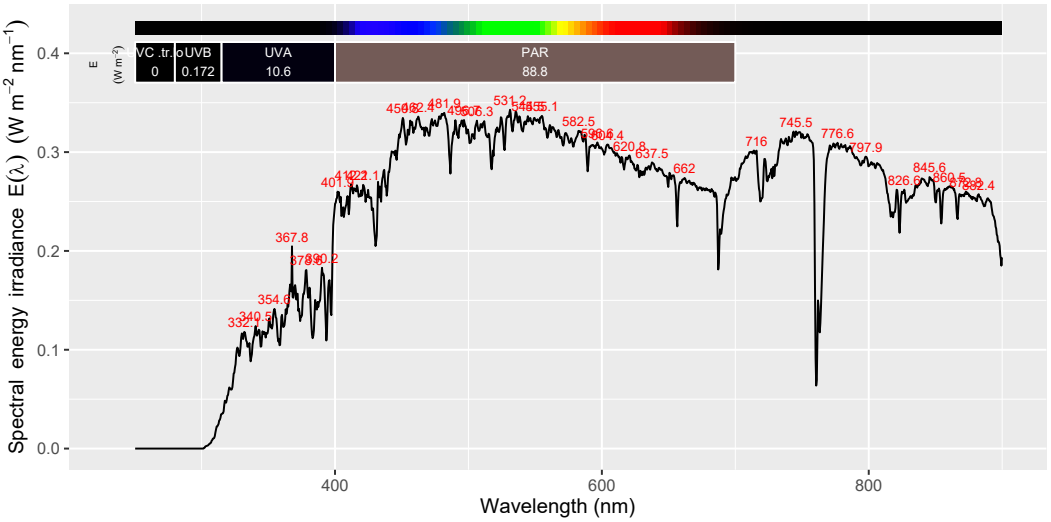


We convert the returned curves into a `source_spct` objects.

```
func_med_FM.spct <-
  source_spct(w.length = attr(gap.mat, "w.length"),
              s.e.irrad = func_med_FM$data[1, ])
func_med_mode.spct <-
  source_spct(w.length = attr(gap.mat, "w.length"),
              s.e.irrad = func_med_mode$data[1, ])
func_med_RP.spct <-
  source_spct(w.length = attr(gap.mat, "w.length"),
              s.e.irrad = func_med_RP$data[1, ])
```

We plot one spectrum using plot method from package 'ggspectra'.

```
plot(func_med_mode.spct)
```



We calculate one summary.

```
q_ratio(func_med_mode.spct, Red("Smith10"), Far_red("Smith10"))

##  Red.Smith10: FarRed.Smith10(q:q)
##                          0.8268562
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

We create a collection of spectra.

```
gap_fda.mspct <- source_mspct(list(med_FM = func_med_FM.spct,
                  med_mode = func_med_mode.spct,
                  med_RP = func_med_RP.spct))
```

Calculate spectral summaries.

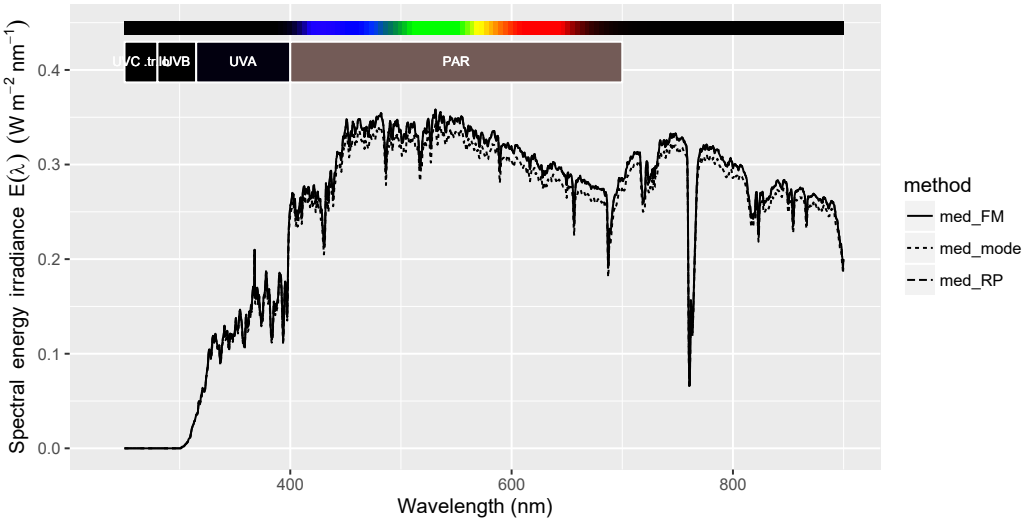
```
ratios <- q_ratio(gap_fda.mspct, Red("Smith10"), Far_red("Smith10"))
names(ratios) <- c("method", "R:FR")
ratios

## # A tibble: 3 x 2
##     method      R:FR
##     <fctr>     <dbl>
## 1   med_FM 0.8334827
## 2 med_mode 0.8268562
## 3   med_RP 0.8334827
```

We bind the three spectra to be able to plot them together.

```
gap_fda.spct <-
  rbindspct(gap_fda.mspct,
            idfactor = "method")
```

We plot three spectra using plot method from package 'ggspectra'.

```
plot(gap_fda.spct,
     annotations = c("color.guide", "boxes", "labels")) +
  aes(linetype = method)
```



19

Importing and exporting 'foreign' data

19.1 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(readr)
library(readxl)
library(photobiology)
library(photobiologyInOut)
#library(ooacquire)
#library(Yoctopuce)
library(lubridate)
```

19.2 Reading and writing common file formats

19.2.1 Task: Read and write text files

19.2.2 Task: Read and write worksheets

19.3 Reading instrument-output files

19.3.1 Task: Import data from Ocean Optics instruments and software

Reading spectral (energy) irradiance from a file saved in Ocean Optics SpectraSuite software, now superseded by OceanView.

```
ooss.spct <- read_oo_ssirrad("inout/spectrum.SSIrrad")
ooss.spct

## Object: source_spct [1,044 x 2]
## Wavelength range 199.08 to 998.61 nm, step 0.72 to 0.81 nm
## Measured on 2013-05-06 15:13:40 UTC
## Time unit 1s
##
## # A tibble: 1,044 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1   199.08    0.0000
## 2   199.89    0.0000
## 3   200.70    0.0000
## 4   201.50    1.3742
## # ... with 1,040 more rows
```

The function accepts several optional arguments. Although the function by default attempts to read all information from the files, values like the date can be overridden and a geocode can be set.

```
ooss1.spct <- read_oo_ssirrad("inout/spectrum.SSIrrad",
                              date = now())
ooss1.spct

## Object: source_spct [1,044 x 2]
## Wavelength range 199.08 to 998.61 nm, step 0.72 to 0.81 nm
## Measured on 2016-07-28 22:18:11 UTC
## Time unit 1s
##
## # A tibble: 1,044 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1   199.08    0.0000
## 2   199.89    0.0000
## 3   200.70    0.0000
## 4   201.50    1.3742
## # ... with 1,040 more rows
```

Files saved by Ocean Optics *Jaz* spectrometers have a slightly different format, and a function different function is to be used.

```
jaz.spct <- read_oo_jazirrad("inout/spectrum.JazIrrad")

## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.032

jaz.spct

## Object: source_spct [2,048 x 2]
## Wavelength range 188.82523 to 1033.1483 nm, step 0.357056 to 0.459625 nm
## Label: File: inout/spectrum.JazIrrad
## Measured on 2015-02-03 09:44:41 UTC
## Time unit 1s
##
## # A tibble: 2,048 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 188.8252         0
## 2 189.2849         0
## 3 189.7444         0
## 4 190.2040         0
## # ... with 2,044 more rows
```

Function `read_oojaz_file` accepts the same arguments as function `read_ooss_file`.

```
jaz1.spct <- read_oo_jazirrad("inout/spectrum.JazIrrad",
                              date = now())

## Warning in range_check(x, strict.range = strict.range): Negative spectral energy
irradiance values; minimun s.e.irrad = -0.032

jaz1.spct
```

```
## Object: source_spct [2,048 x 2]
## Wavelength range 188.82523 to 1033.1483 nm, step 0.357056 to 0.459625 nm
## Label: File: inout/spectrum.JazIrrad
## Measured on 2016-07-28 22:18:11 UTC
## Time unit 1s
##
## # A tibble: 2,048 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1 188.8252         0
## 2 189.2849         0
## 3 189.7444         0
## 4 190.2040         0
## # ... with 2,044 more rows
```

19.3.2 Task: Import data from Avantes instruments and software

```
avantes.spct <- read_avaspec_csv("inout/spectrum-avaspec.csv",
                                 date = now())
avantes.spct
```

```
## Object: source_spct [1,604 x 2]
## Wavelength range 172.485 to 1100.222 nm, step 0.544 to 0.607 nm
## Label: File: inout/spectrum-avaspec.csv
## Measured on 2016-07-28 22:18:11 UTC
## Time unit 1s
##
## # A tibble: 1,604 x 2
##   w.length   s.e.irrad
##      <dbl>       <dbl>
## 1  172.485 9.27919e-12
## 2  173.091 1.10348e-11
## 3  173.697 1.04457e-11
## 4  174.303 8.93041e-12
## # ... with 1,600 more rows
```

19.3.3 Task: Import data from Macam instruments and software

The Macam PC-1900 spectroradiometer and its companion software save data in a simple text file. Data is always stored as spectral (energy) irradiance, so spectral data can be easily decoded. All the files we have tested had the name tag ".DTA".

```
macam.spct <- read_macam_dta("inout/spectrum.DTA")
macam.spct
```

```
## Object: source_spct [151 x 2]
## Wavelength range 250 to 400 nm, step 1 nm
## Label: File: inout/spectrum.DTA
## Measured on 1997-05-19 17:44:58 UTC
## Time unit 1s
##
## # A tibble: 151 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
```

```
## 1      250         0
## 2      251         0
## 3      252         0
## 4      253         0
## # ... with 147 more rows
```

Function `read_macam_dta` accepts the same arguments as function `read_ooss_file`.

```
macam1.spct <- read_macam_dta("inout/spectrum.DTA",
                              date = now())
macam1.spct

## Object: source_spct [151 x 2]
## Wavelength range 250 to 400 nm, step 1 nm
## Label: File: inout/spectrum.DTA
## Measured on 2016-07-28 22:18:11 UTC
## Time unit 1s
##
## # A tibble: 151 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1      250         0
## 2      251         0
## 3      252         0
## 4      253         0
## # ... with 147 more rows
```

19.3.4 Task: Import data from LI-COR instruments and software

The LI-COR LI-1800 spectroradiometer and its companion software can save data either as spectral photon irradiance or spectral (energy) irradiance. As files are labelled accordingly, our function, automatically detects the type of data being read. Be aware that the function is not able to decode the binary files ".DAT". Only ".PRN" as converted by LI-COR's PC1800 software can be decoded.

```
licor.spct <- read_licor_prn("inout/spectrum.PRN")
licor.spct

## Object: source_spct [601 x 2]
## Wavelength range 300 to 900 nm, step 1 nm
## Label: File: inout/spectrum.PRN
## Measured on 0000-08-23 16:32:00 UTC
## Time unit 1s
##
## # A tibble: 601 x 2
##   w.length s.q.irrad
##      <dbl>     <dbl>
## 1      300 1.518e-10
## 2      301 3.355e-10
## 3      302 2.197e-10
## 4      303 3.240e-10
## # ... with 597 more rows
```

Function `read_licor_file` accepts the same arguments as function `read_ooss_file`.

```
licor1.spct <- read_licor_prn("inout/spectrum.PRN",
                              date = now())
licor1.spct

## Object: source_spct [601 x 2]
## Wavelength range 300 to 900 nm, step 1 nm
## Label: File: inout/spectrum.PRN
## Measured on 2016-07-28 22:18:12 UTC
## Time unit 1s
##
## # A tibble: 601 x 2
##   w.length s.q.irrad
##       <dbl>     <dbl>
## 1      300 1.518e-10
## 2      301 3.355e-10
## 3      302 2.197e-10
## 4      303 3.240e-10
## # ... with 597 more rows
```

19.3.5 Task: Import data from Bentham instruments and software

19.4 Acquiring data directly from within R

In this section, the code is not run when compiling the text, as then producing a PDF would require instruments to be available.

19.4.1 Task: Acquiring data from Ocean Optics instruments and software

For the examples in this section to work, you will need to have Java and the OmniDriver runtime installed. In addition examples as shown assume that an Ocean Optics spectrometer is connected. The output will depend on the model(s) and configuration(s) of the instrument(s) connected. The plural is correct, you can acquire spectra from more than one instrument, and from instruments with more than one channel.

Package 'rOmniDriver' is just a thin wrapper on the low-level access functions supplied by the driver. The names for functions in package 'rOminiDriver' are verbose, this is because we have respected the names used in the driver itself, written in Java. Thus was done so that information in the driver documentation can be found easily.

First step is to load the package 'rOmniDriver' which is a low level wrapper on the driver supplied by Ocean Optics for their instruments. The runtime is free, and is all what you need for simple tasks as documentation is available both from Ocean Optics web site and as R help.

```
library(rOmniDrive)
```

After physically connecting the spectrometer through USB, the data connection needs to be initiated and the instrument id obtained. This function returns a 'Java wrapper' object that will be used for all later operations and needs to be saved to variable. The second statement queries the number of spectrometers, or spectrometer modules in the case of the *Jaz*.

```
srs <- init_srs()
num_srs <- number_srs()
```

Indexing starts at zero, contrary to R's way, so the first spectrometer has index '0', the second index '1', etc.

We will now assume that only one spectrometer is attached to the computer, and just rely on the default index value of 0, which always points to the first available spectrometer. The next step, unless we always use the same instrument is to query for a description of the optical bench of the attached instrument.

```
get_name(srs)
get_serial_number(srs)
get_bench(srs)
```

If you are writing a script that should work with different instruments, you may need to query whether a certain function is available or not in the attached instrument. On the other functions like those used for setting the integration time can be just assumed to be always available. Many functions come in pairs of `set` and `get`. The only thing to be careful with is that in some cases, the `set` functions can be silently ignored. For this reason, scripts have to written so that these functions are not assumed to always work. The most important case, setting the integration time, be be easily dealt with in to different ways: 1) being careful the set function is passed as argument an off-range time value, or even more reliably, 2) always using the corresponding get function after each call to set, to obtain the value actually stored in the memory of the spectrometer. Not following these steps can result in errors of any size, and render the data useless.

```
set_integration_time(srs, time.usec = 100)
get_integration_time(srs)
```

We can similarly set the number of scans to average.

```
set_scans_to_avg(srs, 5)
get_scans_to_avg(srs)
```

To obtain data we use function `get_spectrum`

```
counts <- get_spectrum(srs)
```

```
srs_close(srs)
```

More advanced tasks like downloading calibration data from a spectrometer are not yet implemented, but will be added soon.

19.4.2 Task: Acquiring data from sglux instruments and software

19.4.3 Task: Acquiring data from YoctoPuce modules and servers

20

Calibration

21

Simulation

Part V

Catalogue of example data

22

Radiation sources

22.1 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)
library(photobiologySun)
library(photobiologyLamps)
library(photobiologyLEDs)
```

22.2 Introduction

22.3 Data: extraterrestrial solar radiation spectra

22.4 Data: terrestrial solar radiation spectra

- Global irradiance consists of both direct and diffuse components:
  - Direct irradiance is solar radiation that comes in a straight line from the direction of the sun at its current position in the sky.
  - Diffuse irradiance is solar radiation that has been scattered by molecules and particles in the atmosphere or scattered and reflected from the surroundings.
- Two standardization parties commonly referred to, the American Society for Testing and Materials (ASTM) and the International Electrotechnical Commission (IEC) both use the Simple Model of the Atmospheric Radiative Transfer of Sunshine (SMARTS) program to generate terrestrial reference spectra for photovoltaic system performance evaluation and product comparison and hence their reference spectra are essentially the same.
- The standards define global irradiance where the receiving surface is defined in the standards as an inclined plane at 37° tilt toward the equator, facing the sun (i.e., the surface normal points to the sun, at an elevation of 41.81° above the horizon), and expressed as $\mathrm{W\,m^{-2}\,nm^{-1}}$.
- American Society for Testing and Materials (ASTM) defines two standard terrestrial solar spectral irradiance distributions:
  - The AM1.5 Global irradiance spectrum

  - The AM1.5 Direct (+circumsolar) spectrum that is defined for solar concentrator work. It includes the the direct beam from the sun plus the circumsolar component, that results from scattered radiation appearing to come from around the solar disk.

- There is no standard sun spectrum specified separately for plant photobiology or horticulture.
- Plant photobiologists refer to these SMARTS derived spectrum as well.
- The global irradiance spectrum can be considered to be more relevant for plant photobiology and horticulture.

22.5 Data: radiation within plant canopies

22.6 Data: radiation in water bodies

22.7 Data: incandescent lamps

22.8 Data: discharge lamps

22.9 Data: LEDs

23

Optical properties of inanimate objects

23.1 Packages used in this chapter

For accessing the example data listed in this chapter you need first to load the following packages from the library:

```
library(photobiology)
library(photobiologyFilters)
library(photobiologyReflectors)
```

23.2 Introduction

23.3 Data: spectral transmittance of filters

23.4 Data: spectral reflectance of filters

23.5 Data: spectral transmittance of common materials

23.6 Data: spectral reflectance of common materials

24

Example data for organisms

24.1 Plants

24.1.1 Data: Surface properties of organs

24.1.2 Data: Photoreceptors

24.1.3 Data: Photosynthesis

24.1.4 Data: Damage

24.1.5 Data: Metabolites

24.2 Animals, including humans

24.2.1 Data: Surface properties of organs

24.2.2 Data: Photoreceptors

24.2.3 Data: Light driven synthesis

24.2.4 Data: Damage

24.2.5 Data: Metabolites

24.3 Microbes

24.3.1 Data: Photoreceptors

24.3.2 Data: Light driven synthesis

24.3.3 Data: Damage

24.3.4 Data: Metabolites

25

Further reading

25.1 Radiation physics

25.2 Photochemistry

25.3 Photobiology

25.4 Using R

25.5 Programming in R

Glossary

absorbance $A = \log E_0/E_1$, where E_0 is the incident irradiance, and E_1 is the transmitted irradiance. xxi

absorptance radiation that is absorbed by an object, as a fraction of the incident irradiance: $\alpha = E_{\text{abs}}/E_0$, where E_0 is the incident irradiance and E_{abs} is the absorbed irradiance. xxi

biological spectral weighting function a function used to estimate the biological effect of radiation. It is convoluted—i.e. multiplied wavelength by wavelength—with the spectral irradiance of a source of UV radiation to obtain a biologically effective irradiance. xxi

CRAN, Comprehensive R Archive Network A network of software and documentation repositories for R packages and R itself. 40

direct radiation solar radiation that arrives directly at the ground level, without being scattered by gases and particles of the atmosphere. 16, 28

global radiation total solar radiation arriving at ground level. It is the sum of direct and diffuse radiation. 16, *see* direct radiation

isotropic radiation is isotropic when it arrives equally from all directions, e.g. it is completely diffuse. *see* scattered or 'diffuse' radiation

photosynthetic photon flux density another name for 'PAR photon irradiance'. xxii

photosynthetically active radiation radiation driving photosynthesis in higher plants, it describes a wavelength range—i.e. λ =400–700 nm—but does not define whether an energy or photon quantity is being used. xxii

proportional-integral-derivative a *proportional integral derivative* controller (PID controller) is a control loop feedback mechanism. A PID controller calculates an "error" value as the difference between a measured process variable and a desired setpoint. The controller attempts to minimize the error by adjusting the process control inputs. A well tuned PID controller (with correct parameters) minimizes overshoot and transient deviations, by adjusting, for example, the dimming in a modulated system based on the size of the error and the response characteristics of the controlled system. xxii

radiation amplification factor gives the percent change in biologically effective UV irradiance for a 1% change in stratospheric ozone column thickness. Its value varies with the BSWF used in the calculation. xxii

reflectance radiation that is reflected by an object, as a fraction of the incident irradiance: $\rho = E_{\text{rfl}}/E_0$, where E_0 is the incident irradiance and E_{rfl} is the reflected irradiance. xxi

scattered or 'diffuse' radiation solar radiation that arrives at ground level after being scattered by gases and particles of the atmosphere, also called 'diffuse radiation'. 16

transmittance radiation that is transmitted by an object, as a fraction of the incident irradiance: $\tau = E_{\text{trs}}/E_0$, where E_0 is the incident irradiance and E_{trs} is the transmitted irradiance. xxi

Index

Part VI

Appendix

A

Build information

```
Sys.info()
```

```
##        sysname        release        version
##      "Windows"       "10 x64"  "build 10586"
##       nodename        machine          login
##         "MUSTI"       "x86-64"       "aphalo"
##           user effective_user
##       "aphalo"       "aphalo"
```

```
sessionInfo()
```

```
## R version 3.3.1 (2016-06-21)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
## Running under: Windows 10 x64 (build 10586)
##
## 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] splines   grid      methods   stats
## [5] graphics  grDevices utils     datasets
## [9] base
##
## other attached packages:
##  [1] readxl_0.1.1
##  [2] readr_0.2.2
##  [3] fda.usc_1.2.3
##  [4] rpart_4.1-10
##  [5] mgcv_1.8-12
##  [6] nlme_3.1-128
##  [7] MASS_7.3-45
##  [8] fda_2.4.4
##  [9] Matrix_1.2-6
## [10] pavo_0.5-5
## [11] rgl_0.95.1441
## [12] colorSpec_0.5-3
## [13] hyperSpec_0.98-20150304
## [14] mvtnorm_1.0-5
## [15] ggspectra_0.1.7.9002
## [16] lubridate_1.5.6
## [17] photobiologyInOut_0.4.6.9000
## [18] photobiologyReflectors_0.3.2
## [19] photobiologyPlants_0.3.3.9001
## [20] dplyr_0.5.0
```

```
## [21] scales_0.4.0
## [22] caret_6.0-70
## [23] ggplot2_2.1.0
## [24] lattice_0.20-33
## [25] signal_0.7-6
## [26] rootSolve_1.6.6
## [27] rgdal_1.1-10
## [28] raster_2.5-8
## [29] sp_1.2-3
## [30] photobiologyWavebands_0.4.0
## [31] photobiologySun_0.3.7
## [32] photobiology_0.9.8.9001
## [33] knitr_1.13
##
## loaded via a namespace (and not attached):
##  [1] pbkrtest_0.4-6
##  [2] RColorBrewer_1.1-2
##  [3] latex2exp_0.4.0
##  [4] tensorA_0.36
##  [5] tools_3.3.1
##  [6] R6_2.1.2
##  [7] DBI_0.4-1
##  [8] lazyeval_0.2.0
##  [9] colorspace_1.2-6
## [10] nnet_7.3-12
## [11] gridExtra_2.2.1
## [12] bayesm_3.0-2
## [13] compositions_1.40-1
## [14] quantreg_5.26
## [15] formatR_1.4
## [16] photobiologyLamps_0.3.4
## [17] SparseM_1.7
## [18] labeling_0.3
## [19] photobiologyFilters_0.4.2
## [20] DEoptimR_1.0-6
## [21] robustbase_0.92-6
## [22] stringr_1.0.0
## [23] digest_0.6.9
## [24] minqa_1.2.4
## [25] photobiologyLEDs_0.4.1
## [26] jpeg_0.1-8
## [27] lme4_1.1-12
## [28] highr_0.6
## [29] maps_3.1.1
## [30] svUnit_0.7-12
## [31] energy_1.6.2
## [32] car_2.1-2
## [33] magrittr_1.5
## [34] geosphere_1.5-5
## [35] Rcpp_0.12.6
## [36] munsell_0.4.3
## [37] proto_0.3-10
## [38] stringi_1.1.1
## [39] RJSONIO_1.3-0
## [40] plyr_1.8.4
## [41] hsdar_0.4.1
## [42] parallel_3.3.1
## [43] mapproj_1.2-4
## [44] rcdd_1.1-10
## [45] boot_1.3-18
```

```
## [46] rjson_0.2.15
## [47] reshape2_1.4.1
## [48] codetools_0.2-14
## [49] stats4_3.3.1
## [50] magic_1.5-6
## [51] evaluate_0.9
## [52] latticeExtra_0.6-28
## [53] splus2R_1.2-1
## [54] png_0.1-7
## [55] nloptr_1.0.4
## [56] foreach_1.4.3
## [57] RgoogleMaps_1.2.0.7
## [58] MatrixModels_0.4-1
## [59] gtable_0.2.0
## [60] tidyr_0.5.1
## [61] assertthat_0.1
## [62] geometry_0.3-6
## [63] tibble_1.1
## [64] iterators_1.0.8
## [65] ggtern_2.1.4
## [66] ggmap_2.6.1
```